Pentaerithrol, tetrakis-(2-ethylhexanoate)

Other names: 2,2-bis[[(2-ethyl-1-oxohexyl)oxy]methyl]propane-1,3-diyl bis(2-ethylhexanoate)
Pentaerythritol tetra-2-ethylhexanoate
pentaerythritol tetra(2-ethylhexanoate)
Inchi: InChI=1S/C37H68O8/c1-9-17-21-29(13-5)33(38)42-25-37(26-43-34(39)30(14-6)22-18-10
InchiKey: DRRMRHKHTQRWMB-UHFFFAOYSA-N
Formula: C37H68O8
SMILES: CCCCC(CC)C(=O)OCC(COC(=O)C(CC)CCCC)(COC(=O)C(CC)CCCC)COC(=O)C(CC)C
Mol. weight [g/mol]: 640.93
CAS: 7299-99-2

Physical Properties

Property code	Value	Unit	Source
gf	-681.94	kJ/mol	Joback Method
hf	-1816.08	kJ/mol	Joback Method
hfus	81.23	kJ/mol	Joback Method
hvap	131.73	kJ/mol	Joback Method
log10ws	-9.55		Crippen Method
logp	9.011		Crippen Method
mcvol	561.950	ml/mol	McGowan Method
pc	486.23	kPa	Joback Method
tb	1346.13	K	Joback Method
tc	1851.81	K	Joback Method
tf	737.81	K	Joback Method
vc	2.168	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2103.58	J/mol×K	1683.25	Joback Method
cpg	2123.46	J/mol×K	1514.69	Joback Method
cpg	2122.16	J/mol×K	1430.41	Joback Method
cpg	2112.21	J/mol×K	1346.13	Joback Method
cpg	2084.16	J/mol×K	1767.53	Joback Method
cpg	2059.58	J/mol×K	1851.81	Joback Method

cpg	2116.97	J/mol×K	1598.97	Joback Method
dvisc	0.0000090	Pa×s	839.20	Joback Method
dvisc	0.0000044	Pa×s	940.58	Joback Method
dvisc	0.0000024	Pa×s	1041.97	Joback Method
dvisc	0.0000015	Pa×s	1143.36	Joback Method
dvisc	0.0000010	Pa×s	1244.74	Joback Method
dvisc	0.0000007	Pa×s	1346.13	Joback Method
dvisc	0.0000228	Pa×s	737.81	Joback Method
hvapt	126.40	kJ/mol	399.00	NIST Webbook
pvap	6.44e-04	kPa	443.17	Vapor pressure measurements in the range 10-5 Pa to 1 Pa of four pentaerythritol esters Density and vapor liquid equilibria modeling of ester lubricants
pvap	2.87e-04	kPa	433.18	Vapor pressure measurements in the range 10-5 Pa to 1 Pa of four pentaerythritol esters Density and vapor liquid equilibria modeling of ester lubricants
pvap	1.33e-04	kPa	423.40	Vapor pressure measurements in the range 10-5 Pa to 1 Pa of four pentaerythritol esters Density and vapor liquid equilibria modeling of ester lubricants
pvap	5.82e-05	kPa	413.44	Vapor pressure measurements in the range 10-5 Pa to 1 Pa of four pentaerythritol esters Density and vapor liquid equilibria modeling of ester lubricants
pvap	2.37e-05	kPa	403.44	Vapor pressure measurements in the range 10-5 Pa to 1 Pa of four pentaerythritol esters Density and vapor liquid equilibria modeling of ester lubricants

pvap	8.94e-06	kPa	393.56	Vapor pressure measurements in the range 10-5 Pa to 1 Pa of four pentaerythritol esters Density and vapor liquid equilibria modeling of ester lubricants
pvap	3.37e-06	kPa	383.56	Vapor pressure measurements in the range 10-5 Pa to 1 Pa of four pentaerythritol esters Density and vapor liquid equilibria modeling of ester lubricants
pvap	1.07e-06	kPa	373.81	Vapor pressure measurements in the range 10-5 Pa to 1 Pa of four pentaerythritol esters Density and vapor liquid equilibria modeling of ester lubricants
pvap	3.67e-07	kPa	363.89	Vapor pressure measurements in the range 10-5 Pa to 1 Pa of four pentaerythritol esters Density and vapor liquid equilibria modeling of ester lubricants
pvap	1.27e-07	kPa	353.96	Vapor pressure measurements in the range 10-5 Pa to 1 Pa of four pentaerythritol esters Density and vapor liquid equilibria modeling of ester lubricants

Datasets

Mass density, kg/m3

Temperature, K - Liquid	Pressure, kPa - Liquid	Mass density, kg/m3 - Liquid
278.15	100.00	971.86
278.15	1000.00	972.35
278.15	5000.00	974.57
278.15	10000.00	977.26
278.15	15000.00	979.87
278.15	20000.00	982.42
278.15	25000.00	984.85
278.15	30000.00	987.27
278.15	35000.00	989.6
278.15	40000.00	991.89
278.15	45000.00	994.12
283.15	100.00	968.45
283.15	1000.00	968.97
283.15	5000.00	971.24
283.15	10000.00	974.05
283.15	15000.00	976.74
283.15	20000.00	979.35
283.15	25000.00	981.87
283.15	30000.00	984.34
283.15	35000.00	986.75
283.15	40000.00	989.06
283.15	45000.00	991.35
293.15	100.00	961.62
293.15	1000.00	962.16
293.15	5000.00	964.55
293.15	10000.00	967.46
293.15	15000.00	970.3
293.15	20000.00	973.0
293.15	25000.00	975.67
293.15	30000.00	978.27
293.15	35000.00	980.77
293.15	40000.00	983.23
293.15	45000.00	985.61
303.15	100.00	954.72
303.15	1000.00	955.27
303.15	5000.00	957.79
303.15	10000.00	960.83
303.15	15000.00	963.79
303.15	20000.00	966.65
303.15	25000.00	969.41
303.15	30000.00	972.11
303.15	35000.00	974.73
303.15	40000.00	977.27

303.15	45000.00	979.76
313.15	100.00	947.88
313.15	1000.00	948.35
313.15	5000.00	950.98
313.15	10000.00	954.14
313.15	15000.00	957.23
313.15	20000.00	960.21
313.15	25000.00	963.1
313.15	30000.00	965.89
313.15	35000.00	968.62
313.15	40000.00	971.26
313.15	45000.00	973.82
323.15	100.00	940.45
323.15	1000.00	941.25
323.15	5000.00	943.86
323.15	10000.00	947.2
323.15	15000.00	950.44
323.15	20000.00	953.54
323.15	25000.00	956.57
323.15	30000.00	959.48
323.15	35000.00	962.32
323.15	40000.00	965.0
323.15	45000.00	967.75
333.15	100.00	933.58
333.15	1000.00	934.21
333.15	5000.00	937.13
333.15	10000.00	940.66
333.15	15000.00	944.02
333.15	20000.00	947.27
333.15	25000.00	950.4
333.15	30000.00	953.41
333.15	35000.00	956.37
333.15	40000.00	959.21
333.15	45000.00	961.98
343.15	100.00	926.49
343.15	1000.00	927.17
343.15	5000.00	930.23
343.15	10000.00	933.89
343.15	15000.00	937.42
343.15	20000.00	940.81
343.15	25000.00	944.09
343.15	30000.00	947.23
343.15	35000.00	950.27
343.15	40000.00	953.23

343.15	45000.00	956.09
353.15	100.00	919.45
353.15	1000.00	920.14
353.15	5000.00	923.34
353.15	10000.00	927.13
353.15	15000.00	930.84
353.15	20000.00	934.37
353.15	25000.00	937.77
353.15	30000.00	941.05
353.15	35000.00	944.19
353.15	40000.00	947.27
353.15	45000.00	950.24

Reference *https://www.doi.org/10.1021/je049580w*

Sources

Compressed Liquid Densities of Squalane and Pentaerythritol Tetra(2-ethylhexanoate):	https://www.doi.org/10.1021/je049580w
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Solubility of Carbon Dioxide in Two Pentaerythritol Ester Oils between (283 and 338) K:	https://www.doi.org/10.1021/je800178x
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7299992&Units=SI
Vapor pressure measurements in the range 10-5 Pa to 1 Pa of four pentaerythritol esters Density and	https://www.doi.org/10.1016/j.fluid.2007.07.029
Density Measurements under Pressure for Mixtures of Pentaerythritol Ester	https://www.doi.org/10.1021/je700121n
Vapor liquid equilibria modeling of ester lubricants:	
Cubiciane Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Density-Viscosity Relationship:	

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

pc:	Critical Pressure
pvap:	Vapor pressure
rhol:	Liquid Density
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume