

Tetrapropylene glycol, diacetate

Inchi:
InchiKey:
Formula:
SMILES:
Mol. weight [g/mol]:

InChI=1S/C16H30O7/c1-11(7-20-13(3)9-22-15(5)17)19-8-12(2)21-10-14(4)23-16(6)18/h1-16,18-20,22-23,25-26,28-29,31-32H,33-34H2,35-36H3
NTAADJGIMDADQS-UHFFFAOYSA-N
C16H30O7
CC(=O)OCC(C)OCC(C)OCC(C)OCC(C)OC(C)=O
334.41

Physical Properties

Property code	Value	Unit	Source
gf	-708.76	kJ/mol	Joback Method
hf	-1280.95	kJ/mol	Joback Method
hfus	32.24	kJ/mol	Joback Method
hvap	75.20	kJ/mol	Joback Method
log10ws	-1.95		Crippen Method
logp	1.716		Crippen Method
mcvol	268.790	ml/mol	McGowan Method
pc	1391.25	kPa	Joback Method
rinpol	1879.00		NIST Webbook
rinpol	1876.00		NIST Webbook
rinpol	1873.00		NIST Webbook
rinpol	1877.00		NIST Webbook
rinpol	1873.00		NIST Webbook
rinpol	1878.00		NIST Webbook
rinpol	1875.00		NIST Webbook
rinpol	1876.00		NIST Webbook
rinpol	1878.00		NIST Webbook
rinpol	1875.00		NIST Webbook
rinpol	1875.00		NIST Webbook
rinpol	1879.00		NIST Webbook
tb	783.56	K	Joback Method
tc	970.41	K	Joback Method
tf	421.09	K	Joback Method
vc	1.010	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	825.73	J/mol×K	783.56	Joback Method
cpg	842.19	J/mol×K	814.70	Joback Method
cpg	857.59	J/mol×K	845.84	Joback Method
cpg	871.91	J/mol×K	876.98	Joback Method
cpg	885.12	J/mol×K	908.12	Joback Method
cpg	897.21	J/mol×K	939.27	Joback Method
cpg	908.16	J/mol×K	970.41	Joback Method
dvisc	0.0008347	Pa×s	421.09	Joback Method
dvisc	0.0003343	Pa×s	481.50	Joback Method
dvisc	0.0001642	Pa×s	541.91	Joback Method
dvisc	0.0000930	Pa×s	602.33	Joback Method
dvisc	0.0000584	Pa×s	662.74	Joback Method
dvisc	0.0000397	Pa×s	723.15	Joback Method
dvisc	0.0000286	Pa×s	783.56	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R152286&Units=SI

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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