

Pimelic acid, heptyl pentadecyl ester

Inchi: InChI=1S/C29H56O4/c1-3-5-7-9-10-11-12-13-14-15-16-18-23-27-33-29(31)25-21-19-20-
InchiKey: BKSyrTYBzBYGQG-UHFFFAOYSA-N
Formula: C29H56O4
SMILES: CCCCCCCCCCCCCOC(=O)CCCCC(=O)OCCCCCCC
Mol. weight [g/mol]: 468.75

Physical Properties

Property code	Value	Unit	Source
gf	-274.54	kJ/mol	Joback Method
hf	-1131.49	kJ/mol	Joback Method
hfus	76.44	kJ/mol	Joback Method
hvap	98.46	kJ/mol	Joback Method
log10ws	-9.69		Crippen Method
logp	9.085		Crippen Method
mvol	434.350	ml/mol	McGowan Method
pc	654.10	kPa	Joback Method
rinpol	2507.00		NIST Webbook
rinpol	2507.00		NIST Webbook
tb	1015.50	K	Joback Method
tc	1268.62	K	Joback Method
tf	560.91	K	Joback Method
vc	1.708	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1539.74	J/molxK	1015.50	Joback Method
cpg	1635.54	J/molxK	1226.44	Joback Method
cpg	1620.57	J/molxK	1184.25	Joback Method
cpg	1603.59	J/molxK	1142.06	Joback Method
cpg	1584.52	J/molxK	1099.87	Joback Method
cpg	1563.27	J/molxK	1057.69	Joback Method
cpg	1648.61	J/molxK	1268.62	Joback Method
dvisc	0.0000134	Paxs	1015.50	Joback Method

dvisc	0.0000181	Paxs	939.73	Joback Method
dvisc	0.0000258	Paxs	863.97	Joback Method
dvisc	0.0000393	Paxs	788.20	Joback Method
dvisc	0.0000654	Paxs	712.44	Joback Method
dvisc	0.0001230	Paxs	636.67	Joback Method
dvisc	0.0002741	Paxs	560.91	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406521&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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