

Pimelic acid, propyl pentyl ester

Inchi:	InChI=1S/C15H28O4/c1-3-5-9-13-19-15(17)11-8-6-7-10-14(16)18-12-4-2/h3-13H2,1-2H3
InchiKey:	QDWVFMZVHAKGIA-UHFFFAOYSA-N
Formula:	C15H28O4
SMILES:	CCCCCOC(=O)CCCCC(=O)OCCC
Mol. weight [g/mol]:	272.38

Physical Properties

Property code	Value	Unit	Source
gf	-392.42	kJ/mol	Joback Method
hf	-842.53	kJ/mol	Joback Method
hfus	40.18	kJ/mol	Joback Method
hvap	67.30	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	3.623		Crippen Method
mcvol	237.090	ml/mol	McGowan Method
pc	1518.75	kPa	Joback Method
rinpol	1877.00		NIST Webbook
rinpol	1877.00		NIST Webbook
tb	695.18	K	Joback Method
tc	871.05	K	Joback Method
tf	403.13	K	Joback Method
vc	0.923	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	677.29	J/molxK	695.18	Joback Method
cpg	693.41	J/molxK	724.49	Joback Method
cpg	708.76	J/molxK	753.80	Joback Method
cpg	723.36	J/molxK	783.12	Joback Method
cpg	737.19	J/molxK	812.43	Joback Method
cpg	750.28	J/molxK	841.74	Joback Method
cpg	762.62	J/molxK	871.05	Joback Method
dvisc	0.0013699	Paxs	403.13	Joback Method

dvisc	0.0007100	Paxs	451.81	Joback Method
dvisc	0.0004181	Paxs	500.48	Joback Method
dvisc	0.0002705	Paxs	549.15	Joback Method
dvisc	0.0001878	Paxs	597.83	Joback Method
dvisc	0.0001378	Paxs	646.50	Joback Method
dvisc	0.0001056	Paxs	695.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393807&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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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