

Pimelic acid, 2-methylbutyl propyl ester

Inchi:	InChI=1S/C15H28O4/c1-4-11-18-14(16)9-7-6-8-10-15(17)19-12-13(3)5-2/h13H,4-12H2,1
InchiKey:	UDNQFRXNMUZFCN-UHFFFAOYSA-N
Formula:	C15H28O4
SMILES:	CCCOC(=O)CCCCC(=O)OCC(C)CC
Mol. weight [g/mol]:	272.38

Physical Properties

Property code	Value	Unit	Source
gf	-394.86	kJ/mol	Joback Method
hf	-847.81	kJ/mol	Joback Method
hfus	36.66	kJ/mol	Joback Method
hvap	66.91	kJ/mol	Joback Method
log10ws	-3.58		Crippen Method
logp	3.479		Crippen Method
mcvol	237.090	ml/mol	McGowan Method
pc	1528.27	kPa	Joback Method
rinpol	1834.00		NIST Webbook
rinpol	1834.00		NIST Webbook
tb	694.74	K	Joback Method
tc	872.74	K	Joback Method
tf	388.13	K	Joback Method
vc	0.917	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	677.76	J/molxK	694.74	Joback Method
cpg	751.59	J/molxK	843.08	Joback Method
cpg	738.39	J/molxK	813.41	Joback Method
cpg	724.41	J/molxK	783.74	Joback Method
cpg	709.65	J/molxK	754.07	Joback Method
cpg	694.10	J/molxK	724.41	Joback Method
cpg	764.02	J/molxK	872.74	Joback Method
dvisc	0.0000977	Paxs	694.74	Joback Method

dvisc	0.0001300	Paxs	643.64	Joback Method
dvisc	0.0001817	Paxs	592.54	Joback Method
dvisc	0.0002704	Paxs	541.43	Joback Method
dvisc	0.0004373	Paxs	490.33	Joback Method
dvisc	0.0007909	Paxs	439.23	Joback Method
dvisc	0.0016719	Paxs	388.13	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406645&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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