

Pimelic acid, propyl 2,4,4-trimethylpentyl ester

Inchi:	InChI=1S/C18H34O4/c1-6-12-21-16(19)10-8-7-9-11-17(20)22-14-15(2)13-18(3,4)5/h15H
InchiKey:	LJFKMHZLDFNQOC-UHFFFAOYSA-N
Formula:	C18H34O4
SMILES:	CCCOC(=O)CCCCC(=O)OCC(C)CC(C)(C)C
Mol. weight [g/mol]:	314.46

Physical Properties

Property code	Value	Unit	Source
gf	-366.76	kJ/mol	Joback Method
hf	-918.48	kJ/mol	Joback Method
hfus	37.01	kJ/mol	Joback Method
hvap	72.29	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	4.506		Crippen Method
mcvol	279.360	ml/mol	McGowan Method
pc	1251.26	kPa	Joback Method
rinpol	1582.00		NIST Webbook
rinpol	1582.00		NIST Webbook
tb	760.15	K	Joback Method
tc	944.42	K	Joback Method
tf	424.36	K	Joback Method
vc	1.075	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	851.53	J/molxK	760.15	Joback Method
cpg	930.53	J/molxK	913.71	Joback Method
cpg	916.60	J/molxK	883.00	Joback Method
cpg	901.76	J/molxK	852.29	Joback Method
cpg	885.98	J/molxK	821.57	Joback Method
cpg	869.25	J/molxK	790.86	Joback Method
cpg	943.57	J/molxK	944.42	Joback Method
dvisc	0.0000532	Paxs	760.15	Joback Method

dvisc	0.0000729	Paxs	704.18	Joback Method
dvisc	0.0001056	Paxs	648.22	Joback Method
dvisc	0.0001640	Paxs	592.25	Joback Method
dvisc	0.0002793	Paxs	536.29	Joback Method
dvisc	0.0005382	Paxs	480.32	Joback Method
dvisc	0.0012334	Paxs	424.36	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=U406468&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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