

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

Inchi:	InChI=1S/C23H44O4/c1-6-7-8-9-10-14-17-26-21(24)15-12-11-13-16-22(25)27-19-20(2)1
InchiKey:	KGSIQIORKDKRLY-UHFFFAOYSA-N
Formula:	C23H44O4
SMILES:	CCCCCCCCOC(=O)CCCCC(=O)OCC(C)CC(C)(C)C
Mol. weight [g/mol]:	384.59

Physical Properties

Property code	Value	Unit	Source
gf	-324.66	kJ/mol	Joback Method
hf	-1021.68	kJ/mol	Joback Method
hfus	49.96	kJ/mol	Joback Method
hvap	83.42	kJ/mol	Joback Method
log10ws	-6.69		Crippen Method
logp	6.456		Crippen Method
mvol	349.810	ml/mol	McGowan Method
pc	914.39	kPa	Joback Method
rinpol	1836.00		NIST Webbook
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tb	874.55	K	Joback Method
tc	1070.98	K	Joback Method
tf	480.71	K	Joback Method
vc	1.355	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1155.24	J/molxK	874.55	Joback Method
cpg	1240.21	J/molxK	1038.24	Joback Method
cpg	1225.54	J/molxK	1005.50	Joback Method
cpg	1209.75	J/molxK	972.76	Joback Method
cpg	1192.79	J/molxK	940.03	Joback Method
cpg	1174.64	J/molxK	907.29	Joback Method
cpg	1253.82	J/molxK	1070.98	Joback Method
dvisc	0.0000245	Paxs	874.55	Joback Method

dvisc	0.0000339	Paxs	808.91	Joback Method
dvisc	0.0000496	Paxs	743.27	Joback Method
dvisc	0.0000781	Paxs	677.63	Joback Method
dvisc	0.0001358	Paxs	611.99	Joback Method
dvisc	0.0002695	Paxs	546.35	Joback Method
dvisc	0.0006448	Paxs	480.71	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406476&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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