

Pimelic acid, 3-methyl-2-pentyl pentadecyl ester

Inchi:	InChI=1S/C28H54O4/c1-5-7-8-9-10-11-12-13-14-15-16-17-21-24-31-27(29)22-19-18-20-
InchiKey:	DFQWJTQWWXSNMG-UHFFFAOYSA-N
Formula:	C28H54O4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)CCCCC(=O)OC(C)C(C)CC
Mol. weight [g/mol]:	454.73

Physical Properties

Property code	Value	Unit	Source
gf	-287.84	kJ/mol	Joback Method
hf	-1121.41	kJ/mol	Joback Method
hfus	66.80	kJ/mol	Joback Method
hvap	95.46	kJ/mol	Joback Method
log10ws	-9.14		Crippen Method
logp	8.549		Crippen Method
mvol	420.260	ml/mol	McGowan Method
pc	693.25	kPa	Joback Method
rinpol	3062.00		NIST Webbook
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tb	991.74	K	Joback Method
tc	1227.53	K	Joback Method
tf	519.64	K	Joback Method
vc	1.639	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1475.15	J/molxK	991.74	Joback Method
cpg	1497.37	J/molxK	1031.04	Joback Method
cpg	1517.59	J/molxK	1070.34	Joback Method
cpg	1535.87	J/molxK	1109.64	Joback Method
cpg	1552.29	J/molxK	1148.93	Joback Method
cpg	1566.92	J/molxK	1188.23	Joback Method
cpg	1579.83	J/molxK	1227.53	Joback Method
dvisc	0.0004088	Paxs	519.64	Joback Method

dvisc	0.0001579	Paxs	598.32	Joback Method
dvisc	0.0000761	Paxs	677.01	Joback Method
dvisc	0.0000427	Paxs	755.69	Joback Method
dvisc	0.0000267	Paxs	834.37	Joback Method
dvisc	0.0000181	Paxs	913.06	Joback Method
dvisc	0.0000131	Paxs	991.74	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=U406605&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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