

Pimelic acid, octyl pentadecyl ester

Inchi:	InChI=1S/C30H58O4/c1-3-5-7-9-11-12-13-14-15-16-17-19-24-28-34-30(32)26-22-20-21-
InchiKey:	CXFVQZKVVONMQA-UHFFFAOYSA-N
Formula:	C30H58O4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)CCCCC(=O)OCCCCCCCC
Mol. weight [g/mol]:	482.78

Physical Properties

Property code	Value	Unit	Source
gf	-266.12	kJ/mol	Joback Method
hf	-1152.13	kJ/mol	Joback Method
hfus	79.03	kJ/mol	Joback Method
hvap	100.69	kJ/mol	Joback Method
log10ws	-10.11		Crippen Method
logp	9.475		Crippen Method
mvol	448.440	ml/mol	McGowan Method
pc	623.13	kPa	Joback Method
rinpol	3362.00		NIST Webbook
rinpol	3362.00		NIST Webbook
tb	1038.38	K	Joback Method
tc	1305.67	K	Joback Method
tf	572.18	K	Joback Method
vc	1.764	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1605.20	J/molxK	1038.38	Joback Method
cpg	1629.54	J/molxK	1082.93	Joback Method
cpg	1651.34	J/molxK	1127.48	Joback Method
cpg	1670.72	J/molxK	1172.02	Joback Method
cpg	1687.79	J/molxK	1216.57	Joback Method
cpg	1702.67	J/molxK	1261.12	Joback Method
cpg	1715.46	J/molxK	1305.67	Joback Method
dvisc	0.0002389	Paxs	572.18	Joback Method

dvisc	0.0001064	Paxs	649.88	Joback Method
dvisc	0.0000563	Paxs	727.58	Joback Method
dvisc	0.0000337	Paxs	805.28	Joback Method
dvisc	0.0000221	Paxs	882.98	Joback Method
dvisc	0.0000155	Paxs	960.68	Joback Method
dvisc	0.0000114	Paxs	1038.38	Joback Method

Sources

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=U393879&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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