

Pimelic acid, octadecyl 3-methylbutyl ester

Inchi:	InChI=1S/C30H58O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-22-26-33-29(31)23-20
InchiKey:	ZDMYNQXGHKSQNJ-UHFFFAOYSA-N
Formula:	C30H58O4
SMILES:	CCCCCCCCCCCCCCCCCOC(=O)CCCCC(=O)OCCC(C)C
Mol. weight [g/mol]:	482.78

Physical Properties

Property code	Value	Unit	Source
gf	-268.56	kJ/mol	Joback Method
hf	-1157.41	kJ/mol	Joback Method
hfus	75.51	kJ/mol	Joback Method
hvap	100.30	kJ/mol	Joback Method
log10ws	-9.86		Crippen Method
logp	9.331		Crippen Method
mcvol	448.440	ml/mol	McGowan Method
pc	625.63	kPa	Joback Method
rinpol	3342.00		NIST Webbook
rinpol	3342.00		NIST Webbook
tb	1037.94	K	Joback Method
tc	1301.70	K	Joback Method
tf	557.18	K	Joback Method
vc	1.758	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1605.40	J/molxK	1037.94	Joback Method
cpg	1629.35	J/molxK	1081.90	Joback Method
cpg	1650.81	J/molxK	1125.86	Joback Method
cpg	1669.88	J/molxK	1169.82	Joback Method
cpg	1686.68	J/molxK	1213.78	Joback Method
cpg	1701.32	J/molxK	1257.74	Joback Method
cpg	1713.90	J/molxK	1301.70	Joback Method
dvisc	0.0002682	Paxs	557.18	Joback Method

dvisc	0.0001110	Paxs	637.31	Joback Method
dvisc	0.0000560	Paxs	717.43	Joback Method
dvisc	0.0000324	Paxs	797.56	Joback Method
dvisc	0.0000207	Paxs	877.69	Joback Method
dvisc	0.0000143	Paxs	957.81	Joback Method
dvisc	0.0000104	Paxs	1037.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393786&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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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