Pimelic acid, octadecyl pentyl ester

Inchi: InChI=1S/C30H58O4/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-19-24-28-34-30(32)26-2
InchiKey: QHWBXXKWWGKIGK-UHFFFAOYSA-N
Formula: C30H58O4
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)CCCCCC(=O)OCCCCC
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
mcvol	448.440	ml/mol	McGowan Method
pc	623.13	kPa	Joback Method
rinpol	3376.00		NIST Webbook
rinpol	3376.00		NIST Webbook
tb	1038.38	K	Joback Method
tc	1305.67	K	Joback Method
tf	572.18	K	Joback Method
vc	1.764	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0001064	Pa×s	649.88	Joback Method
dvisc	0.0000563	Pa×s	727.58	Joback Method
dvisc	0.0000337	Pa×s	805.28	Joback Method
dvisc	0.0000221	Pa×s	882.98	Joback Method
dvisc	0.0000155	Pa×s	960.68	Joback Method
dvisc	0.0000114	Pa×s	1038.38	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U393823&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

Latest version available from:
https://www.chemeo.com/cid/88-329-0/Pimelic-acid-octadecyl-pentyl-ester.pdf
Generated by Cheméo on 2024-10-12 08:43:43.250032536 +0000 UTC m=+3303485.887001786.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.