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

Inchi: InChI=1S/C30H58O4/c1-6-7-8-9-10-11-12-13-14-15-16-17-21-24-33-28(31)22-19-18-20-

InchiKey: VXIHKKKORHAFTN-UHFFFAOYSA-N

Formula: C30H58O4

SMILES: CCCCCCCCCCCCCCCOC(=O)CCCCCC(=O)OCC(C)CC(C)(C)C

Mol. weight [g/mol]: 482.78

Physical Properties

Property code	Value	Unit	Source
gf	-265.72	kJ/mol	Joback Method
hf	-1166.16	kJ/mol	Joback Method
hfus	68.09	kJ/mol	Joback Method
hvap	99.00	kJ/mol	Joback Method
log10ws	-9.62		Crippen Method
logp	9.187		Crippen Method
mcvol	448.440	ml/mol	McGowan Method
pc	631.61	kPa	Joback Method
rinpol	2439.00		NIST Webbook
rinpol	2439.00		NIST Webbook
tb	1034.71	K	Joback Method
tc	1288.59	K	Joback Method
tf	559.60	K	Joback Method
vc	1.746	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1604.99	J/mol×K	1034.71	Joback Method
cpg	1702.40	J/mol×K	1246.28	Joback Method
cpg	1686.61	J/mol×K	1203.97	Joback Method
cpg	1669.10	J/mol×K	1161.65	Joback Method
cpg	1649.75	J/mol×K	1119.34	Joback Method
cpg	1628.42	J/mol×K	1077.02	Joback Method
cpg	1716.62	J/mol×K	1288.59	Joback Method
dvisc	0.0000078	Pa×s	1034.71	Joback Method

dvisc	0.0000109	Pa×s	955.52	Joback Method
dvisc	0.0000161	Pa×s	876.34	Joback Method
dvisc	0.0000257	Pa×s	797.15	Joback Method
dvisc	0.0000457	Pa×s	717.97	Joback Method
dvisc	0.0000935	Pa×s	638.78	Joback Method
dvisc	0.0002345	Pa×s	559.60	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=U406483&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