Pimelic acid, heptadecyl 2-methylpentyl ester

Inchi: InChI=1S/C30H58O4/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-18-22-26-33-29(31)24-20-1
InchiKey: AFNUKJPCRWRBOV-UHFFFAOYSA-N
Formula: C30H58O4
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)CCCCCC(=O)OCC(C)CCC
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	3305.00		NIST Webbook
rinpol	3305.00		NIST Webbook
tb	1037.94	K	Joback Method
tc	1301.70	K	Joback Method
tf	557.18	K	Joback Method
vc	1.758	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0001110	Pa×s	637.31	Joback Method
dvisc	0.0000560	Pa×s	717.43	Joback Method
dvisc	0.0000324	Pa×s	797.56	Joback Method
dvisc	0.0000207	Pa×s	877.69	Joback Method
dvisc	0.0000143	Pa×s	957.81	Joback Method
dvisc	0.0000104	Pa×s	1037.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406678&Units=SI
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

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