Pimelic acid, hexadecyl 2-methylbutyl ester

Inchi: InChI=1S/C28H54O4/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-21-24-31-27(29)22-19-18-2
InchiKey: DYJVYDDNIDCZEZ-UHFFFAOYSA-N
Formula: C28H54O4
SMILES: CCCCCCCCCCCCCCCCOC(=O)CCCCCC(=O)OCC(C)CC
Mol. weight [g/mol]: 454.73

Physical Properties

Property code	Value	Unit	Source
gf	-285.40	kJ/mol	Joback Method
hf	-1116.13	kJ/mol	Joback Method
hfus	70.33	kJ/mol	Joback Method
hvap	95.85	kJ/mol	Joback Method
log10ws	-9.03		Crippen Method
logp	8.551		Crippen Method
mcvol	420.260	ml/mol	McGowan Method
pc	690.34	kPa	Joback Method
rinpol	3123.00		NIST Webbook
rinpol	3123.00		NIST Webbook
tb	992.18	K	Joback Method
tc	1230.25	K	Joback Method
tf	534.64	K	Joback Method
vc	1.645	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1474.86	J/mol×K	992.18	Joback Method
cpg	1567.75	J/mol×K	1190.58	Joback Method
cpg	1552.94	J/mol×K	1150.90	Joback Method
cpg	1536.31	J/mol×K	1111.22	Joback Method
cpg	1517.80	J/mol×K	1071.54	Joback Method
cpg	1497.34	J/mol×K	1031.86	Joback Method
cpg	1580.84	J/mol×K	1230.25	Joback Method
dvisc	0.0000144	Pa×s	992.18	Joback Method

dvisc	0.0000196	Pa×s	915.92	Joback Method
dvisc	0.0000284	Pa×s	839.67	Joback Method
dvisc	0.0000442	Pa×s	763.41	Joback Method
dvisc	0.0000759	Pa×s	687.15	Joback Method
dvisc	0.0001491	Pa×s	610.90	Joback Method
dvisc	0.0003555	Pa×s	534.64	Joback Method

Sources

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=U406658&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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