Pimelic acid, hexadecyl 3-methyl-2-pentyl ester

Inchi: InChI=1S/C29H56O4/c1-5-7-8-9-10-11-12-13-14-15-16-17-18-22-25-32-28(30)23-20-19-

InchiKey: UEUPVRPMHVMQTJ-UHFFFAOYSA-N

Formula: C29H56O4

SMILES: CCCCCCCCCCCCCCCCOC(=O)CCCCCC(=O)OC(C)C(C)CC

Mol. weight [g/mol]: 468.75

Physical Properties

Property code	Value	Unit	Source
gf	-279.42	kJ/mol	Joback Method
hf	-1142.05	kJ/mol	Joback Method
hfus	69.39	kJ/mol	Joback Method
hvap	97.68	kJ/mol	Joback Method
log10ws	-9.56		Crippen Method
logp	8.939		Crippen Method
mcvol	434.350	ml/mol	McGowan Method
pc	659.49	kPa	Joback Method
rinpol	3165.00		NIST Webbook
rinpol	3165.00		NIST Webbook
tb	1014.62	K	Joback Method
tc	1261.98	K	Joback Method
tf	530.91	K	Joback Method
vc	1.696	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1540.24	J/mol×K	1014.62	Joback Method
cpg	1563.12	J/mol×K	1055.85	Joback Method
cpg	1583.78	J/mol×K	1097.07	Joback Method
cpg	1602.32	J/mol×K	1138.30	Joback Method
cpg	1618.82	J/mol×K	1179.53	Joback Method
cpg	1633.37	J/mol×K	1220.75	Joback Method
cpg	1646.05	J/mol×K	1261.98	Joback Method
dvisc	0.0003537	Pa×s	530.91	Joback Method

dvisc	0.0001359	Pa×s	611.53	Joback Method
dvisc	0.0000652	Pa×s	692.15	Joback Method
dvisc	0.0000365	Pa×s	772.76	Joback Method
dvisc	0.0000228	Pa×s	853.38	Joback Method
dvisc	0.0000154	Pa×s	934.00	Joback Method
dvisc	0.0000111	Pa×s	1014.62	Joback Method

Sources

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=U406606&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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