1,2-Cyclohexanedicarboxylic acid, hexadecyl 5-methoxy-3-methylpentyl ester

Inchi: InChI=1S/C31H58O5/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-19-24-35-30(32)28-20-17-18

InchiKey: UDASPNAIHSYCEG-UHFFFAOYSA-N

Formula: C31H58O5

SMILES: CCCCCCCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OCCC(C)CCOC

Mol. weight [g/mol]: 510.79

Physical Properties

Property code	Value	Unit	Source
gf	-348.40	kJ/mol	Joback Method
hf	-1276.29	kJ/mol	Joback Method
hfus	72.19	kJ/mol	Joback Method
hvap	105.05	kJ/mol	Joback Method
log10ws	-8.78		Crippen Method
logp	8.423		Crippen Method
mcvol	457.540	ml/mol	McGowan Method
pc	644.51	kPa	Joback Method
rinpol	3493.00		NIST Webbook
rinpol	3493.00		NIST Webbook
tb	1098.12	K	Joback Method
tc	1371.10	K	Joback Method
tf	593.82	K	Joback Method
vc	1.764	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1698.32	J/mol×K	1098.12	Joback Method
cpg	1717.97	J/mol×K	1143.62	Joback Method
cpg	1734.37	J/mol×K	1189.11	Joback Method
cpg	1747.61	J/mol×K	1234.61	Joback Method
cpg	1757.77	J/mol×K	1280.11	Joback Method
cpg	1764.95	J/mol×K	1325.60	Joback Method
cpg	1769.22	J/mol×K	1371.10	Joback Method
dvisc	0.0001985	Pa×s	593.82	Joback Method

dvisc	0.0000861	Pa×s	677.87	Joback Method
dvisc	0.0000449	Pa×s	761.92	Joback Method
dvisc	0.0000266	Pa×s	845.97	Joback Method
dvisc	0.0000174	Pa×s	930.02	Joback Method
dvisc	0.0000122	Pa×s	1014.07	Joback Method
dvisc	0.0000090	Pa×s	1098.12	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=U339927&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