1,2-Cyclohexanedicarboxylic acid, 2-methylbutyl octadecyl ester

Inchi: InChI=1S/C31H58O4/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-18-19-22-25-34-30(32)28-2

InchiKey: UTCXGQOZBZBADH-UHFFFAOYSA-N

Formula: C31H58O4

SMILES: CCCCCCCCCCCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OCC(C)CC

Mol. weight [g/mol]: 494.79

Physical Properties

Property code	Value	Unit	Source
gf	-243.40	kJ/mol	Joback Method
hf	-1144.07	kJ/mol	Joback Method
hfus	71.00	kJ/mol	Joback Method
hvap	102.64	kJ/mol	Joback Method
log10ws	-9.69		Crippen Method
logp	9.187		Crippen Method
mcvol	451.670	ml/mol	McGowan Method
pc	650.11	kPa	Joback Method
rinpol	3436.00		NIST Webbook
tb	1075.70	K	Joback Method
tc	1336.51	K	Joback Method
tf	571.59	K	Joback Method
vc	1.746	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1669.67	J/mol×K	1075.70	Joback Method
cpg	1690.84	J/mol×K	1119.17	Joback Method
cpg	1709.28	J/mol×K	1162.64	Joback Method
cpg	1725.09	J/mol×K	1206.10	Joback Method
cpg	1738.36	J/mol×K	1249.57	Joback Method
cpg	1749.22	J/mol×K	1293.04	Joback Method
cpg	1757.75	J/mol×K	1336.51	Joback Method
dvisc	0.0002969	Pa×s	571.59	Joback Method
dvisc	0.0001244	Pa×s	655.61	Joback Method

dvisc	0.0000635	Pa×s	739.63	Joback Method
dvisc	0.0000372	Pa×s	823.64	Joback Method
dvisc	0.0000240	Pa×s	907.66	Joback Method
dvisc	0.0000167	Pa×s	991.68	Joback Method
dvisc	0.0000123	Pa×s	1075.70	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=U339555&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