1,2-Cyclohexanedicarboxylic acid, 3,5-dimethylcyclohexyl pentadecyl ester

Inchi: InChI=1S/C31H56O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-18-21-34-30(32)28-19-16-17-20

InchiKey: WTXCPTWDTSMILA-UHFFFAOYSA-N

Formula: C31H56O4

SMILES: CCCCCCCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OC1CC(C)CC(C)C1

Mol. weight [g/mol]: 492.77

Physical Properties

Property code	Value	Unit	Source
gf	-231.93	kJ/mol	Joback Method
hf	-1125.15	kJ/mol	Joback Method
hfus	68.50	kJ/mol	Joback Method
hvap	102.84	kJ/mol	Joback Method
log10ws	-9.46		Crippen Method
logp	8.795		Crippen Method
mcvol	440.810	ml/mol	McGowan Method
pc	695.81	kPa	Joback Method
rinpol	3391.00		NIST Webbook
rinpol	3391.00		NIST Webbook
tb	1086.35	K	Joback Method
tc	1336.91	K	Joback Method
tf	585.49	K	Joback Method
vc	1.683	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1671.31	J/mol×K	1086.35	Joback Method
cpg	1689.63	J/mol×K	1128.11	Joback Method
cpg	1705.01	J/mol×K	1169.87	Joback Method
cpg	1717.53	J/mol×K	1211.63	Joback Method
cpg	1727.26	J/mol×K	1253.39	Joback Method
cpg	1734.26	J/mol×K	1295.15	Joback Method
cpg	1738.62	J/mol×K	1336.91	Joback Method
dvisc	0.0004021	Pa×s	585.49	Joback Method

dvisc	0.0001919	Pa×s	668.97	Joback Method
dvisc	0.0001079	Pa×s	752.44	Joback Method
dvisc	0.0000681	Pa×s	835.92	Joback Method
dvisc	0.0000467	Pa×s	919.40	Joback Method
dvisc	0.0000341	Pa×s	1002.87	Joback Method
dvisc	0.0000261	Pa×s	1086.35	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=U339856&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