1,2-Cyclohexanedicarboxylic acid, heptadecyl 2-methylcyclohexyl ester

Inchi: InChI=1S/C32H58O4/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-21-26-35-31(33)28-23-18-1

InchiKey: IGDXQEFYAZCORF-UHFFFAOYSA-N

Formula: C32H58O4

SMILES: CCCCCCCCCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OC1CCCCC1C

Mol. weight [g/mol]: 506.80

Physical Properties

Property code	Value	Unit	Source
gf	-215.80	kJ/mol	Joback Method
hf	-1125.45	kJ/mol	Joback Method
hfus	70.02	kJ/mol	Joback Method
hvap	105.38	kJ/mol	Joback Method
log10ws	-10.12		Crippen Method
logp	9.329		Crippen Method
mcvol	454.900	ml/mol	McGowan Method
pc	673.25	kPa	Joback Method
rinpol	3597.00		NIST Webbook
rinpol	3597.00		NIST Webbook
tb	1113.90	K	Joback Method
tc	1376.33	K	Joback Method
tf	601.00	K	Joback Method
vc	1.740	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1731.39	J/mol×K	1113.90	Joback Method
cpg	1793.23	J/mol×K	1332.59	Joback Method
cpg	1786.56	J/mol×K	1288.86	Joback Method
cpg	1777.14	J/mol×K	1245.12	Joback Method
cpg	1764.87	J/mol×K	1201.38	Joback Method
cpg	1749.66	J/mol×K	1157.64	Joback Method
cpg	1797.27	J/mol×K	1376.33	Joback Method
dvisc	0.0000163	Pa×s	1113.90	Joback Method

dvisc	0.0000217	Pa×s	1028.42	Joback Method
dvisc	0.0000303	Pa×s	942.93	Joback Method
dvisc	0.0000454	Pa×s	857.45	Joback Method
dvisc	0.0000742	Pa×s	771.97	Joback Method
dvisc	0.0001373	Pa×s	686.48	Joback Method
dvisc	0.0003026	Pa×s	601.00	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=U339885&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