1,2-Cyclohexanedicarboxylic acid, hexadecyl 4-octyl ester

Inchi: InChI=1S/C32H60O4/c1-4-7-9-10-11-12-13-14-15-16-17-18-19-22-27-35-31(33)29-25-20
InchiKey: BNTGPKZCEXLQFE-UHFFFAOYSA-N
Formula: C32H60O4
SMILES: CCCCCCCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OC(CCC)CCCC
Mol. weight [g/mol]: 508.82

Physical Properties

Property code	Value	Unit	Source
gf	-234.98	kJ/mol	Joback Method
hf	-1164.71	kJ/mol	Joback Method
hfus	73.59	kJ/mol	Joback Method
hvap	104.87	kJ/mol	Joback Method
log10ws	-10.47		Crippen Method
logp	9.719		Crippen Method
mcvol	465.760	ml/mol	McGowan Method
pc	619.41	kPa	Joback Method
rinpol	3652.00		NIST Webbook
rinpol	3652.00		NIST Webbook
tb	1098.58	K	Joback Method
tc	1372.59	K	Joback Method
tf	582.86	K	Joback Method
vc	1.802	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1734.74	J/mol×K	1098.58	Joback Method
cpg	1813.23	J/mol×K	1326.92	Joback Method
cpg	1803.04	J/mol×K	1281.25	Joback Method
cpg	1790.23	J/mol×K	1235.58	Joback Method
cpg	1774.66	J/mol×K	1189.92	Joback Method
cpg	1756.20	J/mol×K	1144.25	Joback Method
cpg	1820.92	J/mol×K	1372.59	Joback Method
dvisc	0.0000105	Pa×s	1098.58	Joback Method

dvisc	0.0000143	Pa×s	1012.63	Joback Method
dvisc	0.0000205	Pa×s	926.67	Joback Method
dvisc	0.0000319	Pa×s	840.72	Joback Method
dvisc	0.0000546	Pa×s	754.77	Joback Method
dvisc	0.0001074	Pa×s	668.81	Joback Method
dvisc	0.0002579	Pa×s	582.86	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=U339530&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