1,2-Cyclohexanedicarboxylic acid, hexadecyl heptyl ester

Inchi: InChI=1S/C31H58O4/c1-3-5-7-9-10-11-12-13-14-15-16-17-19-23-27-35-31(33)29-25-21-

InchiKey: QWYFEBMXIAQWFP-UHFFFAOYSA-N

Formula: C31H58O4

SMILES: CCCCCCCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OCCCCCCC

Mol. weight [g/mol]: 494.79

Physical Properties

Property code	Value	Unit	Source
gf	-240.96	kJ/mol	Joback Method
hf	-1138.79	kJ/mol	Joback Method
hfus	74.53	kJ/mol	Joback Method
hvap	103.03	kJ/mol	Joback Method
log10ws	-9.94		Crippen Method
logp	9.331		Crippen Method
mcvol	451.670	ml/mol	McGowan Method
pc	647.46	kPa	Joback Method
rinpol	3450.00		NIST Webbook
rinpol	3450.00		NIST Webbook
tb	1076.14	K	Joback Method
tc	1339.80	K	Joback Method
tf	586.59	K	Joback Method
vc	1.752	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1669.54	J/mol×K	1076.14	Joback Method
cpg	1691.03	J/mol×K	1120.08	Joback Method
cpg	1709.74	J/mol×K	1164.03	Joback Method
cpg	1725.79	J/mol×K	1207.97	Joback Method
cpg	1739.28	J/mol×K	1251.91	Joback Method
cpg	1750.31	J/mol×K	1295.85	Joback Method
cpg	1759.01	J/mol×K	1339.80	Joback Method
dvisc	0.0002675	Pa×s	586.59	Joback Method

dvisc	0.0001202	Pa×s	668.18	Joback Method
dvisc	0.0000643	Pa×s	749.77	Joback Method
dvisc	0.0000389	Pa×s	831.37	Joback Method
dvisc	0.0000257	Pa×s	912.96	Joback Method
dvisc	0.0000182	Pa×s	994.55	Joback Method
dvisc	0.0000136	Pa×s	1076.14	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=U339544&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