cis-Cyclohex-4-en-1,2-dicarboxylic acid, 2-ethylhexyl hexadecyl ester

Inchi: InChI=1S/C32H58O4/c1-4-7-9-10-11-12-13-14-15-16-17-18-19-22-26-35-31(33)29-24-20

InchiKey: MAXWOIQLPZZMSZ-UHFFFAOYSA-N

Formula: C32H58O4

SMILES: CCCCCCCCCCCCCCCCOC(=O)C1CC=CCC1C(=O)OCC(CC)CCCC

Mol. weight [g/mol]: 506.80

Physical Properties

Property code	Value	Unit	Source
gf	-205.02	kJ/mol	Joback Method
hf	-1106.93	kJ/mol	Joback Method
hfus	74.81	kJ/mol	Joback Method
hvap	105.16	kJ/mol	Joback Method
log10ws	-9.97		Crippen Method
logp	9.353		Crippen Method
mcvol	461.460	ml/mol	McGowan Method
pc	630.66	kPa	Joback Method
rinpol	3396.00		NIST Webbook
rinpol	3396.00		NIST Webbook
tb	1097.74	K	Joback Method
tc	1369.98	K	Joback Method
tf	583.62	K	Joback Method
vc	1.788	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1701.51	J/mol×K	1097.74	Joback Method
cpg	1722.37	J/mol×K	1143.11	Joback Method
cpg	1740.37	J/mol×K	1188.49	Joback Method
cpg	1755.63	J/mol×K	1233.86	Joback Method
cpg	1768.28	J/mol×K	1279.23	Joback Method
cpg	1778.46	J/mol×K	1324.61	Joback Method
cpg	1786.28	J/mol×K	1369.98	Joback Method
dvisc	0.0002618	Pa×s	583.62	Joback Method

dvisc	0.0001118	Pa×s	669.31	Joback Method
dvisc	0.0000579	Pa×s	754.99	Joback Method
dvisc	0.0000343	Pa×s	840.68	Joback Method
dvisc	0.0000224	Pa×s	926.37	Joback Method
dvisc	0.0000157	Pa×s	1012.05	Joback Method
dvisc	0.0000116	Pa×s	1097.74	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=U382643&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