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

Inchi: InChI=1S/C31H56O4/c1-4-7-9-10-11-12-13-14-15-16-17-18-21-25-34-30(32)28-23-19-20
InchiKey: KGCNLHMQBQEJBN-UHFFFAOYSA-N
Formula: C31H56O4
SMILES: CCCCCCCCCCCCCCCCOC(=O)C1CC=CCC1C(=O)OCC(CC)CCCC
Mol. weight [g/mol]: 492.77

Physical Properties

Property code	Value	Unit	Source
gf	-213.44	kJ/mol	Joback Method
hf	-1086.29	kJ/mol	Joback Method
hfus	72.22	kJ/mol	Joback Method
hvap	102.94	kJ/mol	Joback Method
log10ws	-9.55		Crippen Method
logp	8.963		Crippen Method
mcvol	447.370	ml/mol	McGowan Method
pc	662.21	kPa	Joback Method
rinpol	3296.00		NIST Webbook
rinpol	3296.00		NIST Webbook
tb	1074.86	K	Joback Method
tc	1334.18	K	Joback Method
tf	572.35	K	Joback Method
vc	1.732	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1636.73	J/mol×K	1074.86	Joback Method
cpg	1657.29	J/mol×K	1118.08	Joback Method
cpg	1675.23	J/mol×K	1161.30	Joback Method
cpg	1690.68	J/mol×K	1204.52	Joback Method
cpg	1703.72	J/mol×K	1247.74	Joback Method
cpg	1714.47	J/mol×K	1290.96	Joback Method
cpg	1723.04	J/mol×K	1334.18	Joback Method
dvisc	0.0003004	Pa×s	572.35	Joback Method

dvisc	0.0001291	Pa×s	656.10	Joback Method
dvisc	0.0000672	Pa×s	739.85	Joback Method
dvisc	0.0000400	Pa×s	823.61	Joback Method
dvisc	0.0000261	Pa×s	907.36	Joback Method
dvisc	0.0000184	Pa×s	991.11	Joback Method
dvisc	0.0000136	Pa×s	1074.86	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=U382642&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