

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

Inchi:	InChI=1S/C30H54O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-21-24-33-29(31)27-22-19-
InchiKey:	YNJCRRDWHBTSMU-UHFFFAOYSA-N
Formula:	C30H54O4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)C1CC=CCC1C(=O)OCC(CC)CC
Mol. weight [g/mol]:	478.75

Physical Properties

Property code	Value	Unit	Source
gf	-221.86	kJ/mol	Joback Method
hf	-1065.65	kJ/mol	Joback Method
hfus	69.64	kJ/mol	Joback Method
hvap	100.71	kJ/mol	Joback Method
log10ws	-9.13		Crippen Method
logp	8.573		Crippen Method
mcvol	433.280	ml/mol	McGowan Method
pc	696.18	kPa	Joback Method
rinpol	3246.00		NIST Webbook
rinpol	3246.00		NIST Webbook
tb	1051.98	K	Joback Method
tc	1299.91	K	Joback Method
tf	561.08	K	Joback Method
vc	1.675	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1572.08	J/molxK	1051.98	Joback Method
cpg	1592.35	J/molxK	1093.30	Joback Method
cpg	1610.23	J/molxK	1134.62	Joback Method
cpg	1625.81	J/molxK	1175.94	Joback Method
cpg	1639.18	J/molxK	1217.27	Joback Method
cpg	1650.42	J/molxK	1258.59	Joback Method
cpg	1659.63	J/molxK	1299.91	Joback Method
dvisc	0.0003438	Paxs	561.08	Joback Method

dvisc	0.0001489	Paxs	642.90	Joback Method
dvisc	0.0000779	Paxs	724.71	Joback Method
dvisc	0.0000465	Paxs	806.53	Joback Method
dvisc	0.0000305	Paxs	888.35	Joback Method
dvisc	0.0000215	Paxs	970.16	Joback Method
dvisc	0.0000160	Paxs	1051.98	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382818&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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