

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

Inchi:	InChI=1S/C30H54O4/c1-3-5-7-9-10-11-12-13-14-15-16-17-18-22-26-34-30(32)28-24-20-
InchiKey:	UVCRRPGDLOOQUEQ-UHFFFAOYSA-N
Formula:	C30H54O4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)C1CC=CCC1C(=O)OCCCCC
Mol. weight [g/mol]:	478.75

Physical Properties

Property code	Value	Unit	Source
gf	-219.42	kJ/mol	Joback Method
hf	-1060.37	kJ/mol	Joback Method
hfus	73.16	kJ/mol	Joback Method
hvap	101.10	kJ/mol	Joback Method
log10ws	-9.37		Crippen Method
logp	8.717		Crippen Method
mvol	433.280	ml/mol	McGowan Method
pc	693.25	kPa	Joback Method
rinpol	3292.00		NIST Webbook
rinpol	3292.00		NIST Webbook
tb	1052.42	K	Joback Method
tc	1302.58	K	Joback Method
tf	576.08	K	Joback Method
vc	1.681	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1571.89	J/molxK	1052.42	Joback Method
cpg	1592.41	J/molxK	1094.11	Joback Method
cpg	1610.52	J/molxK	1135.81	Joback Method
cpg	1626.32	J/molxK	1177.50	Joback Method
cpg	1639.88	J/molxK	1219.19	Joback Method
cpg	1651.29	J/molxK	1260.89	Joback Method
cpg	1660.66	J/molxK	1302.58	Joback Method
dvisc	0.0003102	Paxs	576.08	Joback Method

dvisc	0.0001439	Paxs	655.47	Joback Method
dvisc	0.0000788	Paxs	734.86	Joback Method
dvisc	0.0000485	Paxs	814.25	Joback Method
dvisc	0.0000326	Paxs	893.64	Joback Method
dvisc	0.0000233	Paxs	973.03	Joback Method
dvisc	0.0000176	Paxs	1052.42	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382672&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

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