cis-Cyclohex-4-en-1,2-dicarboxylic acid, heptadecyl 3-methylbutyl ester

Inchi: InChI=1S/C30H54O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20-24-33-29(31)27-21-18

InchiKey: HIZGXUYEEGVKRA-UHFFFAOYSA-N

Formula: C30H54O4

SMILES: CCCCCCCCCCCCCCCCCCOC(=O)C1CC=CCC1C(=O)OCCC(C)C

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	3257.00		NIST Webbook
rinpol	3257.00		NIST Webbook
tb	1051.98	K	Joback Method
tc	1299.91	K	Joback Method
tf	561.08	K	Joback Method
vc	1.675	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1572.08	J/mol×K	1051.98	Joback Method
cpg	1650.42	J/mol×K	1258.59	Joback Method
cpg	1639.18	J/mol×K	1217.27	Joback Method
cpg	1625.81	J/mol×K	1175.94	Joback Method
cpg	1610.23	J/mol×K	1134.62	Joback Method
cpg	1592.35	J/mol×K	1093.30	Joback Method
cpg	1659.63	J/mol×K	1299.91	Joback Method
dvisc	0.0000160	Pa×s	1051.98	Joback Method

dvisc	0.0000215	Pa×s	970.16	Joback Method
dvisc	0.0000305	Pa×s	888.35	Joback Method
dvisc	0.0000465	Pa×s	806.53	Joback Method
dvisc	0.0000779	Pa×s	724.71	Joback Method
dvisc	0.0001489	Pa×s	642.90	Joback Method
dvisc	0.0003438	Pa×s	561.08	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=U382834&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