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

Inchi: InChI=1S/C29H52O4/c1-4-7-9-10-11-12-13-14-15-16-19-23-32-28(30)26-21-17-18-22-27

InchiKey: JSKYHKQIDMKTLN-UHFFFAOYSA-N

Formula: C29H52O4

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

Mol. weight [g/mol]: 464.72

Physical Properties

Property code	Value	Unit	Source
gf	-230.28	kJ/mol	Joback Method
hf	-1045.01	kJ/mol	Joback Method
hfus	67.05	kJ/mol	Joback Method
hvap	98.48	kJ/mol	Joback Method
log10ws	-8.71		Crippen Method
logp	8.183		Crippen Method
mcvol	419.190	ml/mol	McGowan Method
pc	732.84	kPa	Joback Method
rinpol	3092.00		NIST Webbook
rinpol	3092.00		NIST Webbook
tb	1029.10	K	Joback Method
tc	1267.06	K	Joback Method
tf	549.81	K	Joback Method
vc	1.619	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1507.59	J/mol×K	1029.10	Joback Method
cpg	1586.39	J/mol×K	1227.40	Joback Method
cpg	1574.73	J/mol×K	1187.74	Joback Method
cpg	1561.09	J/mol×K	1148.08	Joback Method
cpg	1545.40	J/mol×K	1108.42	Joback Method
cpg	1527.59	J/mol×K	1068.76	Joback Method
cpg	1596.14	J/mol×K	1267.06	Joback Method
dvisc	0.0000187	Pa×s	1029.10	Joback Method

dvisc	0.0000250	Pa×s	949.22	Joback Method
dvisc	0.0000355	Pa×s	869.34	Joback Method
dvisc	0.0000539	Pa×s	789.45	Joback Method
dvisc	0.0000900	Pa×s	709.57	Joback Method
dvisc	0.0001713	Pa×s	629.69	Joback Method
dvisc	0.0003927	Pa×s	549.81	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382640&Units=SI
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

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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