

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

Inchi:	InChI=1S/C31H56O4/c1-3-5-7-9-11-13-14-15-17-19-23-27-35-31(33)29-25-21-20-24-28(
InchiKey:	MIQIQPAGPCPJAC-UHFFFAOYSA-N
Formula:	C31H56O4
SMILES:	CCCCCCCCCCCCOC(=O)C1CC=CCC1C(=O)OCCCCCCCCC
Mol. weight [g/mol]:	492.77

Physical Properties

Property code	Value	Unit	Source
gf	-211.00	kJ/mol	Joback Method
hf	-1081.01	kJ/mol	Joback Method
hfus	75.75	kJ/mol	Joback Method
hvap	103.32	kJ/mol	Joback Method
log10ws	-9.79		Crippen Method
logp	9.107		Crippen Method
mcvol	447.370	ml/mol	McGowan Method
pc	659.49	kPa	Joback Method
rinpol	3364.00		NIST Webbook
rinpol	3364.00		NIST Webbook
tb	1075.30	K	Joback Method
tc	1337.38	K	Joback Method
tf	587.35	K	Joback Method
vc	1.738	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1636.59	J/molxK	1075.30	Joback Method
cpg	1715.54	J/molxK	1293.70	Joback Method
cpg	1704.60	J/molxK	1250.02	Joback Method
cpg	1691.35	J/molxK	1206.34	Joback Method
cpg	1675.67	J/molxK	1162.66	Joback Method
cpg	1657.45	J/molxK	1118.98	Joback Method
cpg	1724.27	J/molxK	1337.38	Joback Method
dvisc	0.0000150	Paxs	1075.30	Joback Method

dvisc	0.0000200	Paxs	993.98	Joback Method
dvisc	0.0000280	Paxs	912.65	Joback Method
dvisc	0.0000418	Paxs	831.33	Joback Method
dvisc	0.0000682	Paxs	750.00	Joback Method
dvisc	0.0001252	Paxs	668.68	Joback Method
dvisc	0.0002720	Paxs	587.35	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=U382691&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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