cis-Cyclohex-4-en-1,2-dicarboxylic acid, octadecyl pentyl ester

Inchi: InChI=1S/C31H56O4/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-19-23-27-35-31(33)29-2

InchiKey: RKUMSVQAVHURQE-UHFFFAOYSA-N

Formula: C31H56O4

SMILES: CCCCCCCCCCCCCCCCCCCCOC(=O)C1CC=CCC1C(=O)OCCCCC

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	3401.00		NIST Webbook
rinpol	3401.00		NIST Webbook
tb	1075.30	K	Joback Method
tc	1337.38	K	Joback Method
tf	587.35	K	Joback Method
vc	1.738	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0000200	Pa×s	993.98	Joback Method
dvisc	0.0000280	Pa×s	912.65	Joback Method
dvisc	0.0000418	Pa×s	831.33	Joback Method
dvisc	0.0000682	Pa×s	750.00	Joback Method
dvisc	0.0001252	Pa×s	668.68	Joback Method
dvisc	0.0002720	Pa×s	587.35	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382748&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