

1,2-Cyclohexanedicarboxylic acid, 4-octyl pentadecyl ester

Inchi:	InChI=1S/C31H58O4/c1-4-7-9-10-11-12-13-14-15-16-17-18-21-26-34-30(32)28-24-19-20
InchiKey:	WEJIGHUDJNXZBM-UHFFFAOYSA-N
Formula:	C31H58O4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OC(CCC)CCCC
Mol. weight [g/mol]:	494.79

Physical Properties

Property code	Value	Unit	Source
gf	-243.40	kJ/mol	Joback Method
hf	-1144.07	kJ/mol	Joback Method
hfus	71.00	kJ/mol	Joback Method
hvap	102.64	kJ/mol	Joback Method
log10ws	-10.05		Crippen Method
logp	9.329		Crippen Method
mvol	451.670	ml/mol	McGowan Method
pc	650.11	kPa	Joback Method
rinpol	3439.00		NIST Webbook
rinpol	3439.00		NIST Webbook
tb	1075.70	K	Joback Method
tc	1336.51	K	Joback Method
tf	571.59	K	Joback Method
vc	1.746	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1669.67	J/molxK	1075.70	Joback Method
cpg	1690.84	J/molxK	1119.17	Joback Method
cpg	1709.28	J/molxK	1162.64	Joback Method
cpg	1725.09	J/molxK	1206.10	Joback Method
cpg	1738.36	J/molxK	1249.57	Joback Method
cpg	1749.22	J/molxK	1293.04	Joback Method
cpg	1757.75	J/molxK	1336.51	Joback Method
dvisc	0.0002969	Paxs	571.59	Joback Method

dvisc	0.0001244	Paxs	655.61	Joback Method
dvisc	0.0000635	Paxs	739.63	Joback Method
dvisc	0.0000372	Paxs	823.64	Joback Method
dvisc	0.0000240	Paxs	907.66	Joback Method
dvisc	0.0000167	Paxs	991.68	Joback Method
dvisc	0.0000123	Paxs	1075.70	Joback Method

Sources

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=U339529&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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