

Cyclohexanecarboxylic acid, 4-methoxy-, oct-3-en-2-yl ester

Inchi:	InChI=1S/C16H28O3/c1-4-5-6-7-8-13(2)19-16(17)14-9-11-15(18-3)12-10-14/h7-8,13-15H
InchiKey:	HFKFWRJBXAKLLU-BQYQJAHWSA-N
Formula:	C16H28O3
SMILES:	CCCCC=CC(C)OC(=O)C1CCC(OC)CC1
Mol. weight [g/mol]:	268.39

Physical Properties

Property code	Value	Unit	Source
gf	-160.56	kJ/mol	Joback Method
hf	-604.67	kJ/mol	Joback Method
hfus	30.76	kJ/mol	Joback Method
hvap	62.47	kJ/mol	Joback Method
log10ws	-4.20		Crippen Method
logp	3.870		Crippen Method
mcvol	234.450	ml/mol	McGowan Method
pc	1609.00	kPa	Joback Method
rinpol	1837.00		NIST Webbook
rinpol	1837.00		NIST Webbook
tb	682.79	K	Joback Method
tc	881.41	K	Joback Method
tf	347.53	K	Joback Method
vc	0.879	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	682.51	J/molxK	682.79	Joback Method
cpg	773.16	J/molxK	848.31	Joback Method
cpg	757.26	J/molxK	815.20	Joback Method
cpg	740.27	J/molxK	782.10	Joback Method
cpg	722.16	J/molxK	749.00	Joback Method
cpg	702.91	J/molxK	715.89	Joback Method
cpg	787.98	J/molxK	881.41	Joback Method
dvisc	0.0000958	Paxs	682.79	Joback Method

dvisc	0.0001276	Paxs	626.91	Joback Method
dvisc	0.0001799	Paxs	571.04	Joback Method
dvisc	0.0002730	Paxs	515.16	Joback Method
dvisc	0.0004588	Paxs	459.28	Joback Method
dvisc	0.0008903	Paxs	403.41	Joback Method
dvisc	0.0021380	Paxs	347.53	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=U406991&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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