

Cyclohexanecarboxylic acid, 4-methoxy-, octyl ester

Inchi:	InChI=1S/C16H30O3/c1-3-4-5-6-7-8-13-19-16(17)14-9-11-15(18-2)12-10-14/h14-15H,3-
InchiKey:	PQCARJULYDCJSR-UHFFFAOYSA-N
Formula:	C16H30O3
SMILES:	CCCCCCCCOC(=O)C1CCC(OC)CC1
Mol. weight [g/mol]:	270.41

Physical Properties

Property code	Value	Unit	Source
gf	-238.34	kJ/mol	Joback Method
hf	-716.61	kJ/mol	Joback Method
hfus	34.08	kJ/mol	Joback Method
hvap	62.90	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	4.095		Crippen Method
mvol	238.750	ml/mol	McGowan Method
pc	1534.26	kPa	Joback Method
rinpol	1945.00		NIST Webbook
rinpol	1945.00		NIST Webbook
tb	679.07	K	Joback Method
tc	868.14	K	Joback Method
tf	367.61	K	Joback Method
vc	0.905	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	703.83	J/molxK	679.07	Joback Method
cpg	724.26	J/molxK	710.58	Joback Method
cpg	743.61	J/molxK	742.09	Joback Method
cpg	761.90	J/molxK	773.61	Joback Method
cpg	779.12	J/molxK	805.12	Joback Method
cpg	795.29	J/molxK	836.63	Joback Method
cpg	810.41	J/molxK	868.14	Joback Method
dvisc	0.0018288	Paxs	367.61	Joback Method

dvisc	0.0008768	Paxs	419.52	Joback Method
dvisc	0.0004943	Paxs	471.43	Joback Method
dvisc	0.0003122	Paxs	523.34	Joback Method
dvisc	0.0002142	Paxs	575.25	Joback Method
dvisc	0.0001565	Paxs	627.16	Joback Method
dvisc	0.0001199	Paxs	679.07	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406196&Units=SI
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

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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