

Cyclohexane,1-(1,1-dimethylethyl)-4-methoxy-cis-

Inchi:	InChI=1S/C11H22O/c1-11(2,3)9-5-7-10(12-4)8-6-9/h9-10H,5-8H2,1-4H3/t9-,10+
InchiKey:	XMLDPBGRPWQRBE-AOOOYVTPSA-N
Formula:	C11H22O
SMILES:	COC1CCC(C(C)(C)C)CC1
Mol. weight [g/mol]:	170.29
CAS:	15875-99-7

Physical Properties

Property code	Value	Unit	Source
gf	-43.68	kJ/mol	Joback Method
hf	-377.36	kJ/mol	Joback Method
hfus	10.93	kJ/mol	Joback Method
hvap	41.31	kJ/mol	Joback Method
ie	9.36 ± 0.02	eV	NIST Webbook
log10ws	-3.04		Crippen Method
logp	3.238		Crippen Method
mcvol	160.860	ml/mol	McGowan Method
pc	2267.57	kPa	Joback Method
tb	485.15	K	Joback Method
tc	690.68	K	Joback Method
tf	241.52	K	Joback Method
vc	0.591	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	377.78	J/molxK	485.15	Joback Method
cpg	399.45	J/molxK	519.40	Joback Method
cpg	420.00	J/molxK	553.66	Joback Method
cpg	439.46	J/molxK	587.91	Joback Method
cpg	457.85	J/molxK	622.17	Joback Method
cpg	475.22	J/molxK	656.42	Joback Method
cpg	491.58	J/molxK	690.68	Joback Method
dvisc	0.0058275	Paxs	241.52	Joback Method

dvisc	0.0022656	Paxs	282.12	Joback Method
dvisc	0.0011172	Paxs	322.73	Joback Method
dvisc	0.0006452	Paxs	363.33	Joback Method
dvisc	0.0004161	Paxs	403.94	Joback Method
dvisc	0.0002907	Paxs	444.54	Joback Method
dvisc	0.0002157	Paxs	485.15	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=C15875997&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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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