Cyclohexane,1-(1,1-dimethylethyl)-3-methoxy-4-m

Inchi: InChI=1S/C12H22O/c1-9-6-7-10(12(2,3)4)8-11(9)13-5/h10-11H,1,6-8H2,2-5H3/t10-,11-/m
InchiKey: DUVGSEXMTVWEHI-GHMZBOCLSA-N
Formula: C12H22O
SMILES: C=C1CCC(C(C)(C)C)CC1OC
Mol. weight [g/mol]: 182.30
CAS: 68211-39-2

Physical Properties

Property code	Value	Unit	Source
gf	17.82	kJ/mol	Joback Method
hf	-313.76	kJ/mol	Joback Method
hfus	12.36	kJ/mol	Joback Method
hvap	43.70	kJ/mol	Joback Method
ie	8.97 ± 0.02	eV	NIST Webbook
ie	8.97 ± 0.05	eV	NIST Webbook
log10ws	-3.31		Crippen Method
logp	3.404		Crippen Method
mcvol	170.650	ml/mol	McGowan Method
pc	2110.00	kPa	Joback Method
tb	507.19	K	Joback Method
tc	711.61	K	Joback Method
tf	266.47	K	Joback Method
vc	0.630	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.35	J/mol×K	507.19	Joback Method
cpg	503.65	J/mol×K	677.54	Joback Method
cpg	486.83	J/mol×K	643.47	Joback Method
cpg	469.01	J/mol×K	609.40	Joback Method
cpg	450.17	J/mol×K	575.33	Joback Method
cpg	430.30	J/mol×K	541.26	Joback Method
cpg	519.50	J/mol×K	711.61	Joback Method

dvisc	0.0002119	Pa×s	507.19	Joback Method
dvisc	0.0002745	Pa×s	467.07	Joback Method
dvisc	0.0003732	Pa×s	426.95	Joback Method
dvisc	0.0005408	Pa×s	386.83	Joback Method
dvisc	0.0008540	Pa×s	346.71	Joback Method
dvisc	0.0015197	Pa×s	306.59	Joback Method
dvisc	0.0032171	Pa×s	266.47	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C68211392&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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