

Cyclohexene,3-(1,1-dimethylethyl)-6-methoxy-tran

Inchi:	InChI=1S/C11H20O/c1-11(2,3)9-5-7-10(12-4)8-6-9/h5,7,9-10H,6,8H2,1-4H3/t9-,10-/m0/s
InchiKey:	XSCJYACJCMFFJY-UWVGGRQHSA-N
Formula:	C11H20O
SMILES:	COC1C=CC(C(C)(C)C)CC1
Mol. weight [g/mol]:	168.28
CAS:	71555-64-1

Physical Properties

Property code	Value	Unit	Source
gf	-13.72	kJ/mol	Joback Method
hf	-319.58	kJ/mol	Joback Method
hfus	12.15	kJ/mol	Joback Method
hvap	41.61	kJ/mol	Joback Method
ie	8.97 ± 0.02	eV	NIST Webbook
log10ws	-2.89		Crippen Method
logp	3.014		Crippen Method
mcvol	156.560	ml/mol	McGowan Method
pc	2347.36	kPa	Joback Method
tb	484.31	K	Joback Method
tc	691.89	K	Joback Method
tf	242.28	K	Joback Method
vc	0.577	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	361.36	J/molxK	484.31	Joback Method
cpg	381.88	J/molxK	518.91	Joback Method
cpg	401.30	J/molxK	553.50	Joback Method
cpg	419.66	J/molxK	588.10	Joback Method
cpg	436.99	J/molxK	622.70	Joback Method
cpg	453.31	J/molxK	657.30	Joback Method
cpg	468.65	J/molxK	691.89	Joback Method
dvisc	0.0046036	Paxs	242.28	Joback Method

dvisc	0.0019142	Paxs	282.62	Joback Method
dvisc	0.0009910	Paxs	322.96	Joback Method
dvisc	0.0005938	Paxs	363.30	Joback Method
dvisc	0.0003942	Paxs	403.63	Joback Method
dvisc	0.0002819	Paxs	443.97	Joback Method
dvisc	0.0002131	Paxs	484.31	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C71555641&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
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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