Cyclohexanol, 2-methoxy-, (1R,2R)-rel-

Other names: Cyclohexanol,2-methoxy-,trans-
Inchi: InChI=1S/C7H14O2/c1-9-7-5-3-2-4-6(7)8/h6-8H,2-5H2,1H3/t6-,7-/m0/s1
InchiKey: DCQQZLGQRIVCNH-BQBZGAKWSA-N
Formula: C7H14O2
SMILES: COC1CCCCC1O
Mol. weight [g/mol]: 130.18
CAS: 7429-40-5

Physical Properties

Property code	Value	Unit	Source
gf	-217.02	kJ/mol	Joback Method
hf	-438.28	kJ/mol	Joback Method
hfus	12.07	kJ/mol	Joback Method
hvap	50.39	kJ/mol	Joback Method
ie	9.69	eV	NIST Webbook
log10ws	-1.22		Crippen Method
logp	0.936		Crippen Method
mcvol	110.370	ml/mol	McGowan Method
pc	3704.46	kPa	Joback Method
tb	489.04	K	Joback Method
tc	680.38	K	Joback Method
tf	254.84	K	Joback Method
vc	0.397	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.97	J/mol×K	489.04	Joback Method
cpg	319.75	J/mol×K	648.49	Joback Method
cpg	308.16	J/mol×K	616.60	Joback Method
cpg	295.99	J/mol×K	584.71	Joback Method
cpg	283.24	J/mol×K	552.82	Joback Method
cpg	269.90	J/mol×K	520.93	Joback Method
cpg	330.76	J/mol×K	680.38	Joback Method

dvisc	0.0001684	Pa×s	489.04	Joback Method
dvisc	0.0002713	Pa×s	450.01	Joback Method
dvisc	0.0004785	Pa×s	410.97	Joback Method
dvisc	0.0009505	Pa×s	371.94	Joback Method
dvisc	0.0022178	Pa×s	332.91	Joback Method
dvisc	0.0064812	Pa×s	293.87	Joback Method
dvisc	0.0263065	Pa×s	254.84	Joback Method

Sources

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=C7429405&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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