

Cyclohexanol, 2-methyl-, trans-(.+/-.)-

Inchi:	InChI=1S/C7H14O/c1-6-4-2-3-5-7(6)8/h6-8H,2-5H2,1H3/t6-,7-/m0/s1
InchiKey:	NDVWOBYBJYUSMF-BQBZGAKWSA-N
Formula:	C7H14O
SMILES:	CC1CCCCC1O
Mol. weight [g/mol]:	114.19
CAS:	615-39-4

Physical Properties

Property code	Value	Unit	Source
gf	-112.02	kJ/mol	Joback Method
hf	-306.06	kJ/mol	Joback Method
hfus	10.88	kJ/mol	Joback Method
hvap	47.97	kJ/mol	Joback Method
log10ws	-1.78		Crippen Method
logp	1.557		Crippen Method
mcvol	104.500	ml/mol	McGowan Method
pc	3782.33	kPa	Joback Method
tb	439.20	K	NIST Webbook
tc	659.09	K	Joback Method
tf	232.61	K	Joback Method
vc	0.379	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	231.22	J/molxK	466.62	Joback Method
cpg	296.01	J/molxK	627.01	Joback Method
cpg	284.31	J/molxK	594.94	Joback Method
cpg	271.99	J/molxK	562.86	Joback Method
cpg	259.05	J/molxK	530.78	Joback Method
cpg	245.46	J/molxK	498.70	Joback Method
cpg	307.10	J/molxK	659.09	Joback Method
dvisc	0.0002179	Paxs	466.62	Joback Method
dvisc	0.0003597	Paxs	427.62	Joback Method

dvisc	0.0006569	Paxs	388.62	Joback Method
dvisc	0.0013721	Paxs	349.62	Joback Method
dvisc	0.0034480	Paxs	310.61	Joback Method
dvisc	0.0112900	Paxs	271.61	Joback Method
dvisc	0.0550246	Paxs	232.61	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	351.20	K	2.70	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C615394&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume

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