

1,2-Cycloheptanediol, trans-

Other names:	trans-cycloheptane-1,2-diol
Inchi:	InChI=1S/C7H14O2/c8-6-4-2-1-3-5-7(6)9/h6-9H,1-5H2
InchiKey:	DCYPPXGEIQTVPY-UHFFFAOYSA-N
Formula:	C7H14O2
SMILES:	OC1CCCCC1O
Mol. weight [g/mol]:	130.18
CAS:	13553-19-0

Physical Properties

Property code	Value	Unit	Source
gf	-260.94	kJ/mol	Joback Method
hf	-464.45	kJ/mol	Joback Method
hfus	12.87	kJ/mol	Joback Method
hvap	64.83	kJ/mol	Joback Method
log10ws	-1.40		Crippen Method
logp	0.672		Crippen Method
mccvol	110.370	ml/mol	McGowan Method
pc	4391.59	kPa	Joback Method
tb	563.07	K	Joback Method
tc	751.50	K	Joback Method
tf	289.91	K	Joback Method
vc	0.390	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	287.46	J/molxK	563.07	Joback Method
cpg	300.23	J/molxK	594.48	Joback Method
cpg	312.37	J/molxK	625.88	Joback Method
cpg	323.89	J/molxK	657.29	Joback Method
cpg	334.79	J/molxK	688.69	Joback Method
cpg	345.09	J/molxK	720.10	Joback Method
cpg	354.78	J/molxK	751.50	Joback Method
dvisc	0.0891453	Paxs	289.91	Joback Method

dvisc	0.0108501	Paxs	335.44	Joback Method
dvisc	0.0021846	Paxs	380.96	Joback Method
dvisc	0.0006193	Paxs	426.49	Joback Method
dvisc	0.0002239	Paxs	472.02	Joback Method
dvisc	0.0000968	Paxs	517.54	Joback Method
dvisc	0.0000479	Paxs	563.07	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13553190&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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