

2,3,4,7-Tetrahydrooxepin-2-ol

Inchi:	InChI=1S/C6H10O2/c7-6-4-2-1-3-5-8-6/h1,3,6-7H,2,4-5H2
InchiKey:	JXMYHVAAOAIWGIK-UHFFFAOYSA-N
Formula:	C6H10O2
SMILES:	OC1CCC=CCO1
Mol. weight [g/mol]:	114.14
CAS:	41793-28-6

Physical Properties

Property code	Value	Unit	Source
gf	-180.99	kJ/mol	Joback Method
hf	-345.46	kJ/mol	Joback Method
hfus	14.32	kJ/mol	Joback Method
hvap	51.03	kJ/mol	Joback Method
log10ws	-1.04		Crippen Method
logp	0.671		Crippen Method
mcvol	91.980	ml/mol	McGowan Method
pc	4789.21	kPa	Joback Method
tb	478.79	K	Joback Method
tc	682.81	K	Joback Method
tf	249.39	K	Joback Method
vc	0.323	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	200.52	J/molxK	478.79	Joback Method
cpg	254.96	J/molxK	648.81	Joback Method
cpg	245.29	J/molxK	614.80	Joback Method
cpg	235.02	J/molxK	580.80	Joback Method
cpg	224.14	J/molxK	546.80	Joback Method
cpg	212.64	J/molxK	512.79	Joback Method
cpg	264.06	J/molxK	682.81	Joback Method
dvisc	0.0001800	Paxs	478.79	Joback Method
dvisc	0.0003136	Paxs	440.56	Joback Method

dvisc	0.0006073	Paxs	402.32	Joback Method
dvisc	0.0013512	Paxs	364.09	Joback Method
dvisc	0.0036267	Paxs	325.86	Joback Method
dvisc	0.0126560	Paxs	287.62	Joback Method
dvisc	0.0647900	Paxs	249.39	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C41793286&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
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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