

1,2,3,4-Tetrahydronaphthalene-cis-2,3-diol

Inchi:	InChI=1S/C10H12O2/c11-9-5-7-3-1-2-4-8(7)6-10(9)12/h1-4,9-12H,5-6H2/t9-,10+
InchiKey:	DHTGPMXCRKCPTP-AOOOYVTPSA-N
Formula:	C10H12O2
SMILES:	OC1Cc2ccccc2CC1O
Mol. weight [g/mol]:	164.20
CAS:	35583-15-4

Physical Properties

Property code	Value	Unit	Source
chs	-5228.70 ± 0.80	kJ/mol	NIST Webbook
gf	-96.60	kJ/mol	Joback Method
hf	-282.83	kJ/mol	Joback Method
hfus	20.59	kJ/mol	Joback Method
hvap	73.93	kJ/mol	Joback Method
log10ws	-1.72		Crippen Method
logp	0.507		Crippen Method
mcvol	128.880	ml/mol	McGowan Method
pc	4130.29	kPa	Joback Method
tb	650.56	K	Joback Method
tc	850.86	K	Joback Method
tf	373.22	K	Joback Method
vc	0.473	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.49	J/molxK	650.56	Joback Method
cpg	361.80	J/molxK	683.94	Joback Method
cpg	372.40	J/molxK	717.33	Joback Method
cpg	382.33	J/molxK	750.71	Joback Method
cpg	391.64	J/molxK	784.09	Joback Method
cpg	400.35	J/molxK	817.47	Joback Method
cpg	408.51	J/molxK	850.86	Joback Method
dvisc	0.0052728	Paxs	373.22	Joback Method

dvisc	0.0015606	Paxs	419.44	Joback Method
dvisc	0.0005882	Paxs	465.67	Joback Method
dvisc	0.0002644	Paxs	511.89	Joback Method
dvisc	0.0001357	Paxs	558.11	Joback Method
dvisc	0.0000771	Paxs	604.34	Joback Method
dvisc	0.0000475	Paxs	650.56	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C35583154&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

chs:	Standard solid enthalpy of combustion
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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