

Dihydrocuminic alcohol

Inchi:	InChI=1S/C10H16O/c1-8(2)10-5-3-9(7-11)4-6-10/h3,5,8,11H,4,6-7H2,1-2H3
InchiKey:	HBKLBUNCSHWKO-UHFFFAOYSA-N
Formula:	C10H16O
SMILES:	CC(C)C1=CC=C(CO)CC1
Mol. weight [g/mol]:	152.23
CAS:	1335-14-4

Physical Properties

Property code	Value	Unit	Source
gf	-33.12	kJ/mol	Joback Method
hf	-239.96	kJ/mol	Joback Method
hfus	14.65	kJ/mol	Joback Method
hvap	56.79	kJ/mol	Joback Method
log10ws	-2.63		Crippen Method
logp	2.281		Crippen Method
mcvol	138.170	ml/mol	McGowan Method
pc	3093.29	kPa	Joback Method
rinpol	1286.00		NIST Webbook
rinpol	1286.00		NIST Webbook
ripol	1981.00		NIST Webbook
tb	552.44	K	Joback Method
tc	748.10	K	Joback Method
tf	286.46	K	Joback Method
vc	0.514	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	330.66	J/molxK	552.44	Joback Method
cpg	344.29	J/molxK	585.05	Joback Method
cpg	357.21	J/molxK	617.66	Joback Method
cpg	369.45	J/molxK	650.27	Joback Method
cpg	381.03	J/molxK	682.88	Joback Method
cpg	391.98	J/molxK	715.49	Joback Method

cpg	402.32	J/mol×K	748.10	Joback Method
dvisc	0.0168754	Paxs	286.46	Joback Method
dvisc	0.0039809	Paxs	330.79	Joback Method
dvisc	0.0013212	Paxs	375.12	Joback Method
dvisc	0.0005536	Paxs	419.45	Joback Method
dvisc	0.0002739	Paxs	463.78	Joback Method
dvisc	0.0001533	Paxs	508.11	Joback Method
dvisc	0.0000941	Paxs	552.44	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1335144&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
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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