

Dihydrocuminic alcohol, acetate

Inchi:	InChI=1S/C12H18O2/c1-9(2)12-6-4-11(5-7-12)8-14-10(3)13/h4,7,9H,5-6,8H2,1-3H3
InchiKey:	CHRLYELMWCUABI-UHFFFAOYSA-N
Formula:	C12H18O2
SMILES:	CC(=O)OCC1=CCC(C(C)C)=CC1
Mol. weight [g/mol]:	194.27

Physical Properties

Property code	Value	Unit	Source
gf	-113.38	kJ/mol	Joback Method
hf	-373.81	kJ/mol	Joback Method
hfus	18.53	kJ/mol	Joback Method
hvap	53.72	kJ/mol	Joback Method
log10ws	-3.07		Crippen Method
logp	2.852		Crippen Method
mcvol	167.920	ml/mol	McGowan Method
pc	2412.37	kPa	Joback Method
rinpol	1418.00		NIST Webbook
tb	582.31	K	Joback Method
tc	791.69	K	Joback Method
tf	320.34	K	Joback Method
vc	0.631	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	414.22	J/mol×K	582.31	Joback Method
cpg	430.61	J/mol×K	617.21	Joback Method
cpg	446.13	J/mol×K	652.10	Joback Method
cpg	460.78	J/mol×K	687.00	Joback Method
cpg	474.59	J/mol×K	721.90	Joback Method
cpg	487.56	J/mol×K	756.80	Joback Method
cpg	499.71	J/mol×K	791.69	Joback Method
dvisc	0.0024629	Pa×s	320.34	Joback Method
dvisc	0.0011981	Pa×s	364.00	Joback Method

dvisc	0.0006801	Pa×s	407.66	Joback Method
dvisc	0.0004308	Pa×s	451.32	Joback Method
dvisc	0.0002958	Pa×s	494.99	Joback Method
dvisc	0.0002158	Pa×s	538.65	Joback Method
dvisc	0.0001651	Pa×s	582.31	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R129949&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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