Dihydropinol

Inchi: InChI=1S/C10H18O/c1-7-4-5-8-6-9(7)11-10(8,2)3/h7-9H,4-6H2,1-3H3/t7?,8-,9-/m1/s1
InchiKey: MGRKVRJGCZXQGW-CFCGPWAMSA-N
Formula: C10H18O
SMILES: CC1CCC2CC1OC2(C)C
Mol. weight [g/mol]: 154.25

Physical Properties

Property code	Value	Unit	Source
gf	23.59	kJ/mol	Joback Method
hf	-273.89	kJ/mol	Joback Method
hfus	17.55	kJ/mol	Joback Method
hvap	40.77	kJ/mol	Joback Method
log10ws	-2.63		Crippen Method
logp	2.600		Crippen Method
mcvol	135.910	ml/mol	McGowan Method
pc	2775.92	kPa	Joback Method
rinpol	1088.00		NIST Webbook
rinpol	1088.00		NIST Webbook
tb	468.07	K	Joback Method
tc	680.83	K	Joback Method
tf	273.29	K	Joback Method
vc	0.510	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	321.13	J/mol×K	468.07	Joback Method
cpg	341.43	J/mol×K	503.53	Joback Method
cpg	360.35	J/mol×K	538.99	Joback Method
cpg	378.00	J/mol×K	574.45	Joback Method
cpg	394.53	J/mol×K	609.91	Joback Method
cpg	410.06	J/mol×K	645.37	Joback Method
cpg	424.71	J/mol×K	680.83	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R324802&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
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