7-Hydroxy-6,7-dihydronerol

Other names: nerol hydrate
Inchi: InChI=1S/C10H20O2/c1-9(6-8-11)5-4-7-10(2,3)12/h6,11-12H,4-5,7-8H2,1-3H3/b9-6-
InchiKey: JFIQWLBNEDZWHF-TWGQIWQCSA-N
Formula: C10H20O2
SMILES: CC(=CCO)CCCC(C)(C)O
Mol. weight [g/mol]: 172.26

Physical Properties

Property code	Value	Unit	Source
gf	-165.81	kJ/mol	Joback Method
hf	-455.51	kJ/mol	Joback Method
hfus	21.31	kJ/mol	Joback Method
hvap	69.95	kJ/mol	Joback Method
log10ws	-2.50		Crippen Method
logp	1.866		Crippen Method
mcvol	159.200	ml/mol	McGowan Method
pc	2718.33	kPa	Joback Method
ripol	2275.00		NIST Webbook
ripol	2268.00		NIST Webbook
tb	613.37	K	Joback Method
tc	783.82	K	Joback Method
tf	307.48	K	Joback Method
vc	0.604	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	423.91	J/mol×K	613.37	Joback Method
cpg	435.51	J/mol×K	641.78	Joback Method
cpg	446.53	J/mol×K	670.19	Joback Method
cpg	457.00	J/mol×K	698.59	Joback Method
cpg	466.95	J/mol×K	727.00	Joback Method
cpg	476.43	J/mol×K	755.41	Joback Method
cpg	485.46	J/mol×K	783.82	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R329887&Units=SI

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume