8-Hydroxytheaspirane

Inchi: InChI=1S/C13H22O2/c1-9-7-11(14)8-12(3,4)13(9)6-5-10(2)15-13/h7,10-11,14H,5-6,8H2,
InchiKey: AVMRWEITZUAUJV-UHFFFAOYSA-N
Formula: C13H22O2
SMILES: CC1=CC(O)CC(C)(C)C12CCC(C)O2
Mol. weight [g/mol]: 210.31

Physical Properties

Property code	Value	Unit	Source
gf	-97.33	kJ/mol	Joback Method
hf	-438.81	kJ/mol	Joback Method
hfus	19.74	kJ/mol	Joback Method
hvap	64.27	kJ/mol	Joback Method
log10ws	-3.35		Crippen Method
logp	2.661		Crippen Method
mcvol	179.750	ml/mol	McGowan Method
pc	2555.92	kPa	Joback Method
rinpol	1397.00		NIST Webbook
rinpol	1389.00		NIST Webbook
rinpol	1424.00		NIST Webbook
rinpol	1378.00		NIST Webbook
tb	641.81	K	Joback Method
tc	854.83	K	Joback Method
tf	398.06	K	Joback Method
vc	0.665	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	520.06	J/mol×K	641.81	Joback Method
cpg	537.98	J/mol×K	677.31	Joback Method
cpg	555.09	J/mol×K	712.82	Joback Method
cpg	571.59	J/mol×K	748.32	Joback Method
cpg	587.68	J/mol×K	783.82	Joback Method
cpg	603.57	J/mol×K	819.32	Joback Method

cpg	619.44	J/mol×K	854.83	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R217264&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