8,9-dehydrotheaspirone

Inchi: InChI=1S/C13H18O2/c1-9-6-5-7-12(3,4)13(9)8-11(14)10(2)15-13/h5-7,10H,8H2,1-4H3
InchiKey: XGVYEIAYIQAWHE-UHFFFAOYSA-N
Formula: C13H18O2
SMILES: CC1=CC=CC(C)(C)C12CC(=O)C(C)O2
Mol. weight [g/mol]: 206.28

Physical Properties

Property code	Value	Unit	Source
gf	-45.43	kJ/mol	Joback Method
hf	-346.16	kJ/mol	Joback Method
hfus	15.31	kJ/mol	Joback Method
hvap	52.44	kJ/mol	Joback Method
log10ws	-3.11		Crippen Method
logp	2.645		Crippen Method
mcvol	171.150	ml/mol	McGowan Method
pc	2587.22	kPa	Joback Method
rinpol	1518.00		NIST Webbook
rinpol	1518.00		NIST Webbook
tb	621.28	K	Joback Method
tc	868.40	K	Joback Method
tf	410.46	K	Joback Method
vc	0.640	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	465.99	J/mol×K	621.28	Joback Method
cpg	485.43	J/mol×K	662.47	Joback Method
cpg	503.85	J/mol×K	703.65	Joback Method
cpg	521.52	J/mol×K	744.84	Joback Method
cpg	538.72	J/mol×K	786.03	Joback Method
cpg	555.71	J/mol×K	827.22	Joback Method
cpg	572.77	J/mol×K	868.40	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=R225339&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume