theaspirone

Inchi: InChI=1S/C13H20O2/c1-9-7-11(14)8-12(3,4)13(9)6-5-10(2)15-13/h7,10H,5-6,8H2,1-4H3
InchiKey: AXQMCYYCOKLZPP-UHFFFAOYSA-N
Formula: C13H20O2
SMILES: CC1=CC(=O)CC(C)(C)C12CCC(C)O2
Mol. weight [g/mol]: 208.30

Physical Properties

Property code	Value	Unit	Source
gf	-75.39	kJ/mol	Joback Method
hf	-403.94	kJ/mol	Joback Method
hfus	14.09	kJ/mol	Joback Method
hvap	52.15	kJ/mol	Joback Method
log10ws	-3.26		Crippen Method
logp	2.869		Crippen Method
mcvol	175.450	ml/mol	McGowan Method
pc	2495.01	kPa	Joback Method
ripol	2128.00		NIST Webbook
ripol	2128.00		NIST Webbook
tb	622.12	K	Joback Method
tc	866.82	K	Joback Method
tf	409.70	K	Joback Method
vc	0.654	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	487.52	J/mol×K	622.12	Joback Method
cpg	508.16	J/mol×K	662.90	Joback Method
cpg	527.73	J/mol×K	703.69	Joback Method
cpg	546.49	J/mol×K	744.47	Joback Method
cpg	564.71	J/mol×K	785.25	Joback Method
cpg	582.66	J/mol×K	826.03	Joback Method
cpg	600.58	J/mol×K	866.82	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=R320904&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