Nortricyclone

Inchi: InChI=1S/C7H8O/c8-7-3-1-4-5(2-3)6(4)7/h3-6H,1-2H2
InchiKey: ITDQUAQMICQLER-UHFFFAOYSA-N
Formula: C7H8O
SMILES: O=C1C2CC3C(C2)C13
Mol. weight [g/mol]: 108.14
CAS: 695-05-6

Physical Properties

Property code	Value	Unit	Source
gf	84.21	kJ/mol	Joback Method
hf	-115.13	kJ/mol	Joback Method
hfus	13.07	kJ/mol	Joback Method
hvap	34.51	kJ/mol	Joback Method
ie	9.01	eV	NIST Webbook
log10ws	-0.75		Crippen Method
logp	0.841		Crippen Method
mcvol	78.480	ml/mol	McGowan Method
pc	4173.09	kPa	Joback Method
tb	434.39	K	Joback Method
tc	649.94	K	Joback Method
tf	293.49	K	Joback Method
vc	0.321	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	179.92	J/mol×K	434.39	Joback Method
cpg	193.91	J/mol×K	470.32	Joback Method
cpg	206.86	J/mol×K	506.24	Joback Method
cpg	218.85	J/mol×K	542.17	Joback Method
cpg	229.95	J/mol×K	578.09	Joback Method
cpg	240.26	J/mol×K	614.02	Joback Method
cpg	249.84	J/mol×K	649.94	Joback Method

Sources

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=C695056&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume