

Spiro[benzofuran-3(2h),4'-piperidine]-2-one, 5-methyl-

Inchi:	InChI=1S/C13H15NO2/c1-9-2-3-11-10(8-9)13(12(15)16-11)4-6-14-7-5-13/h2-3,8,14H,4-7
InchiKey:	WFCYFCTWZRFSNC-UHFFFAOYSA-N
Formula:	C13H15NO2
SMILES:	Cc1ccc2c(c1)C1(CCNCC1)C(=O)O2
Mol. weight [g/mol]:	217.26
CAS:	116633-09-1

Physical Properties

Property code	Value	Unit	Source
gf	130.25	kJ/mol	Joback Method
hf	-161.09	kJ/mol	Joback Method
hfus	24.47	kJ/mol	Joback Method
hvap	62.98	kJ/mol	Joback Method
log10ws	-2.55		Crippen Method
logp	1.535		Crippen Method
mcvol	165.970	ml/mol	McGowan Method
pc	3356.75	kPa	Joback Method
tb	703.73	K	Joback Method
tc	972.71	K	Joback Method
tf	544.53	K	Joback Method
vc	0.618	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	471.89	J/molxK	703.73	Joback Method
cpg	489.72	J/molxK	748.56	Joback Method
cpg	506.61	J/molxK	793.39	Joback Method
cpg	522.80	J/molxK	838.22	Joback Method
cpg	538.52	J/molxK	883.05	Joback Method
cpg	553.99	J/molxK	927.88	Joback Method
cpg	569.47	J/molxK	972.71	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C116633091&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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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