3H-1,4-Benzodiazepin-2-one, 1,2-dihydro-

Inchi: InChI=1S/C9H8N2O/c12-9-6-10-5-7-3-1-2-4-8(7)11-9/h1-5H,6H2,(H,11,12)
InchiKey: UDLAUVFRZXIQJS-UHFFFAOYSA-N
Formula: C9H8N2O
SMILES: O=C1CN=Cc2ccccc2N1
Mol. weight [g/mol]: 160.17
CAS: 16780-62-4

Physical Properties

Property code	Value	Unit	Source
gf	283.80	kJ/mol	Joback Method
hf	105.65	kJ/mol	Joback Method
hfus	21.04	kJ/mol	Joback Method
hvap	56.64	kJ/mol	Joback Method
ie	7.80	eV	NIST Webbook
log10ws	-1.22		Crippen Method
logp	1.058		Crippen Method
mcvol	120.280	ml/mol	McGowan Method
pc	4717.12	kPa	Joback Method
tb	626.16	K	Joback Method
tc	904.60	K	Joback Method
tf	490.82	K	Joback Method
vc	0.453	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	303.21	J/mol×K	626.16	Joback Method
cpg	318.98	J/mol×K	672.57	Joback Method
cpg	333.46	J/mol×K	718.97	Joback Method
cpg	346.63	J/mol×K	765.38	Joback Method
cpg	358.47	J/mol×K	811.79	Joback Method
cpg	368.97	J/mol×K	858.19	Joback Method
cpg	378.08	J/mol×K	904.60	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=C16780624&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