3H-1,4-Benzodiazepin-2-one, 1,2-dihydro-5-methyl-

Inchi: InChI=1S/C10H10N2O/c1-7-8-4-2-3-5-9(8)12-10(13)6-11-7/h2-5H,6H2,1H3,(H,12,13)
InchiKey: DIDPQMKDRMWTTD-UHFFFAOYSA-N
Formula: C10H10N2O
SMILES: CC1=NCC(O)=Nc2ccccc21
Mol. weight [g/mol]: 174.20
CAS: 70656-87-0

Physical Properties

Property code	Value	Unit	Source
gf	317.76	kJ/mol	Joback Method
hf	138.48	kJ/mol	Joback Method
hfus	24.20	kJ/mol	Joback Method
hvap	72.36	kJ/mol	Joback Method
ie	7.80	eV	NIST Webbook
log10ws	-1.82		Crippen Method
logp	2.097		Crippen Method
mcvol	134.370	ml/mol	McGowan Method
pc	4368.40	kPa	Joback Method
tb	687.67	K	Joback Method
tc	929.40	K	Joback Method
tf	487.00	K	Joback Method
vc	0.518	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	375.21	J/mol×K	687.67	Joback Method
cpg	388.45	J/mol×K	727.96	Joback Method
cpg	400.60	J/mol×K	768.25	Joback Method
cpg	411.66	J/mol×K	808.53	Joback Method
cpg	421.63	J/mol×K	848.82	Joback Method
cpg	430.54	J/mol×K	889.11	Joback Method
cpg	438.38	J/mol×K	929.40	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C70656870&Units=SI
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

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

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