2,3-Dihydro-4-methyl-1H-1,5-benzodiazepin-2-one

Other names: 2H-1,5-Benzodiazepin-2-one, 1,3-dihydro-4-methyl-
4-Methyl-1,5-benzo-diazepin-2-one
1,3-dihydro-4-methyl-2H-1,5-benzodiazepin-2-one
Inchi: InChI=1S/C10H10N2O/c1-7-6-10(13)12-9-5-3-2-4-8(9)11-7/h2-5H,6H2,1H3,(H,12,13)
InchiKey: AFHSLLLKMSITIA-UHFFFAOYSA-N
Formula: C10H10N2O
SMILES: CC1=Nc2ccccc2N=C(O)C1
Mol. weight [g/mol]: 174.20
CAS: 6276-48-8

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
log10ws	-2.32		Crippen Method
logp	2.771		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

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=C6276488&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume