1,5-Dimethylbiuret

Inchi: InChI=1S/C4H9N3O2/c1-5-3(8)7-4(9)6-2/h1-2H3,(H3,5,6,7,8,9)
InchiKey: BEVVHEBDWYSLRT-UHFFFAOYSA-N
Formula: C4H9N3O2
SMILES: CNC(=O)NC(=O)NC
Mol. weight [g/mol]: 131.13
CAS: 16791-94-9

Physical Properties

Property code	Value	Unit	Source
gf	-6.87	kJ/mol	Joback Method
hf	-190.64	kJ/mol	Joback Method
hfus	24.61	kJ/mol	Joback Method
hvap	57.30	kJ/mol	Joback Method
log10ws	-0.57		Crippen Method
logp	-0.745		Crippen Method
mcvol	100.300	ml/mol	McGowan Method
pc	4842.69	kPa	Joback Method
tb	549.17	K	Joback Method
tc	749.39	K	Joback Method
tf	392.68	K	Joback Method
vc	0.377	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	233.03	J/mol×K	549.17	Joback Method
cpg	241.78	J/mol×K	582.54	Joback Method
cpg	250.06	J/mol×K	615.91	Joback Method
cpg	257.87	J/mol×K	649.28	Joback Method
cpg	265.21	J/mol×K	682.65	Joback Method
cpg	272.12	J/mol×K	716.02	Joback Method
cpg	278.59	J/mol×K	749.39	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=C16791949&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
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