

hydroxyurea

Inchi: InChI=1S/CH4N2O2/c2-1(4)3-5/h5H,(H3,2,3,4)
InchiKey: VSNHCAURESNICA-UHFFFAOYSA-N
Formula: CH4N2O2
SMILES: NC(=O)NO
Mol. weight [g/mol]: 76.05

Physical Properties

Property code	Value	Unit	Source
gf	-152.36	kJ/mol	Joback Method
hf	-241.52	kJ/mol	Joback Method
hfus	14.33	kJ/mol	Joback Method
hvap	58.32	kJ/mol	Joback Method
log10ws	1.12		Aqueous Solubility Prediction Method
logp	-0.956		Crippen Method
mcvol	52.350	ml/mol	McGowan Method
pc	8432.26	kPa	Joback Method
tb	491.03	K	Joback Method
tc	685.25	K	Joback Method
tf	415.65	K	Aqueous Solubility Prediction Method
vc	0.180	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	109.52	J/mol×K	491.03	Joback Method
cpg	113.54	J/mol×K	523.40	Joback Method
cpg	117.37	J/mol×K	555.77	Joback Method
cpg	120.98	J/mol×K	588.14	Joback Method
cpg	124.41	J/mol×K	620.51	Joback Method
cpg	127.64	J/mol×K	652.88	Joback Method
cpg	130.68	J/mol×K	685.25	Joback Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

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

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