

dimethylurea

Other names:	Urea, N,N-dimethyl-
Inchi:	InChI=1S/C3H8N2O/c1-4-3(6)5-2/h1-2H3,(H2,4,5,6)
InchiKey:	MGJKQDOBUOMPEZ-UHFFFAOYSA-N
Formula:	C3H8N2O
SMILES:	CNC(=O)NC
Mol. weight [g/mol]:	88.11
CAS:	1320-50-9

Physical Properties

Property code	Value	Unit	Source
chs	-1997.40 ± 0.40	kJ/mol	NIST Webbook
gf	24.24	kJ/mol	Joback Method
hf	-110.89	kJ/mol	Joback Method
hfs	-326.50 ± 0.40	kJ/mol	NIST Webbook
hfus	15.32	kJ/mol	Joback Method
hvap	41.89	kJ/mol	Joback Method
log10ws	-0.21		Crippen Method
logp	-0.455		Crippen Method
mcvol	74.660	ml/mol	McGowan Method
pc	4980.35	kPa	Joback Method
tb	422.25	K	Joback Method
tc	612.72	K	Joback Method
tf	278.82	K	Joback Method
vc	0.280	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	143.48	J/mol×K	422.25	Joback Method
cpg	151.21	J/mol×K	453.99	Joback Method
cpg	158.59	J/mol×K	485.74	Joback Method
cpg	165.65	J/mol×K	517.48	Joback Method
cpg	172.37	J/mol×K	549.23	Joback Method
cpg	178.78	J/mol×K	580.97	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1320509&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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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