

Imidodicarbonic diamide

Other names:	Allophanamide
	Allophanic acid amide
	Allophanimidic acid
	Biuret
	Carbamylurea
	Dicarbamylamine
	Isobiuret
	Urea, (aminocarbonyl)-
	Ureidoformamide
	L-101
Inchi:	NSC 8020
	InChI=1S/C2H5N3O2/c3-1(6)5-2(4)7/h(H5,3,4,5,6,7)
InchiKey:	OHJMTUPIZMNBFR-UHFFFAOYSA-N
Formula:	C2H5N3O2
SMILES:	NC(=O)NC(N)=O
Mol. weight [g/mol]:	103.08
CAS:	108-19-0

Physical Properties

Property code	Value	Unit	Source
chs	-938.00 ± 2.10	kJ/mol	NIST Webbook
gf	-69.59	kJ/mol	Joback Method
hf	-437.00 ± 2.80	kJ/mol	NIST Webbook
hfs	-563.70 ± 2.10	kJ/mol	NIST Webbook
hfus	19.63	kJ/mol	Joback Method
hsub	126.70 ± 1.90	kJ/mol	NIST Webbook
hvap	61.26	kJ/mol	Joback Method
log10ws	-0.22		Crippen Method
logp	-1.267		Crippen Method
mcvol	72.120	ml/mol	McGowan Method
pc	7470.22	kPa	Joback Method
ss	146.10	J/mol×K	NIST Webbook
ss	146.10	J/mol×K	NIST Webbook
tb	548.13	K	Joback Method
tc	773.15	K	Joback Method
tf	431.34	K	Joback Method
vc	0.253	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	162.19	J/mol×K	548.13	Joback Method
cpg	168.05	J/mol×K	585.63	Joback Method
cpg	173.53	J/mol×K	623.14	Joback Method
cpg	178.65	J/mol×K	660.64	Joback Method
cpg	183.39	J/mol×K	698.14	Joback Method
cpg	187.78	J/mol×K	735.64	Joback Method
cpg	191.83	J/mol×K	773.15	Joback Method
cps	131.30	J/mol×K	298.15	NIST Webbook
cps	131.30	J/mol×K	298.15	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C108190&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
cps:	Solid phase 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
hsub:	Enthalpy of sublimation 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
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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