

Glycoluril

Other names:	Acetyleneurea Acetylene diurein Imidazo[4,5-d]imidazole-2,5(1H,3H)-dione, tetrahydro- Acetylene carbamide Acetylenediurea Acetylenediureine Diurea glyoxalate Glyoxalbiuret Glyoxaldiureine Glyoxaldiurene Tetrahydroimidazo(4,5-d)imidazole-2,5(1H,3H)-dione Tetrahydroimidaz(d)imidazole-2,5-(1H,3H)-dione NSC 2765 perhydroimidazo[4,5-d]imidazole-2,5-dione
Inchi:	InChI=1S/C4H6N4O2/c9-3-5-1-2(7-3)8-4(10)6-1/h1-2H,(H2,5,7,9)(H2,6,8,10)
InchiKey:	VPVSTMAPERLKKM-UHFFFAOYSA-N
Formula:	C4H6N4O2
SMILES:	O=C1NC2NC(=O)NC2N1
Mol. weight [g/mol]:	142.12
CAS:	496-46-8

Physical Properties

Property code	Value	Unit	Source
chs	-1938.70 ± 1.90	kJ/mol	NIST Webbook
gf	185.76	kJ/mol	Joback Method
hf	-116.77	kJ/mol	Joback Method
hfs	-492.80 ± 1.90	kJ/mol	NIST Webbook
hfus	35.57	kJ/mol	Joback Method
hvap	60.19	kJ/mol	Joback Method
log10ws	-0.76		Crippen Method
logp	-1.736		Crippen Method
mcvol	88.560	ml/mol	McGowan Method
pc	7943.54	kPa	Joback Method
tb	642.78	K	Joback Method
tc	925.14	K	Joback Method
tf	720.24	K	Joback Method
vc	0.320	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	236.25	J/mol×K	642.78	Joback Method
cpg	249.67	J/mol×K	689.84	Joback Method
cpg	262.24	J/mol×K	736.90	Joback Method
cpg	273.87	J/mol×K	783.96	Joback Method
cpg	284.44	J/mol×K	831.02	Joback Method
cpg	293.83	J/mol×K	878.08	Joback Method
cpg	301.93	J/mol×K	925.14	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C496468&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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