2,4,5-Trioxoimidazolidine

Other names:	2,4,5-Imidazolinetrione
	Imidazole-trione
	Imidazolidinetrione
	Oxalylurea
	Parabanic acid
	Trioxoimidazolidine
Inchi:	InChI=1S/C3H2N2O3/c6-1-2(7)5-3(8)4-1/h(H2,4,5,6,7,8)
InchiKey:	ZFLIKDUSUDBGCD-UHFFFAOYSA-N
Formula:	C3H2N2O3
SMILES:	O=C1NC(=O)C(=O)N1
Mol. weight [g/mol]:	114.06
CAS:	120-89-8

Physical Properties

Property code	Value	Unit	Source
gf	-173.71	kJ/mol	Joback Method
hf	-361.91	kJ/mol	Joback Method
hfus	2.10	kJ/mol	Structural studies of cyclic ureas: 2. Enthalpy of formation of parabanic acid
hsub	119.40 ± 0.60	kJ/mol	NIST Webbook
hvap	49.09	kJ/mol	Joback Method
ie	10.67	eV	NIST Webbook
log10ws	-0.40		Estimated Solubility Method
log10ws	-0.40		Aqueous Solubility Prediction Method
logp	-1.648		Crippen Method
mcvol	66.940	ml/mol	McGowan Method
pc	7721.75	kPa	Joback Method
tb	588.55	K	Joback Method
tc	866.86	K	Joback Method
tf	553.43	K	Joback Method
vc	0.240	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	147.22	J/mol×K	588.55	Joback Method
cpg	157.14	J/mol×K	634.94	Joback Method
cpg	166.79	J/mol×K	681.32	Joback Method
cpg	175.96	J/mol×K	727.71	Joback Method
cpg	184.49	J/mol×K	774.09	Joback Method
cpg	192.18	J/mol×K	820.48	Joback Method
cpg	198.84	J/mol×K	866.86	Joback Method
hsubt	114.60 ± 0.60	kJ/mol	393.50	NIST Webbook

Sources

Structural studies of cyclic ureas: 2. Enthalpy of formation of parabanic acid:	https://www.doi.org/10.1016/j.jct.2008.05.006
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C120898&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
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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