

nitrourea

Inchi:	InChI=1S/CH3N3O3/c2-1(5)3-4(6)7/h(H3,2,3,5)
InchiKey:	CMUOJBJRZUHRMU-UHFFFAOYSA-N
Formula:	CH3N3O3
SMILES:	NC(=O)N[N+](=O)[O-]
Mol. weight [g/mol]:	105.05
CAS:	556-89-8

Physical Properties

Property code	Value	Unit	Source
chs	-541.41	kJ/mol	NIST Webbook
gf	20.01	kJ/mol	Joback Method
hf	-100.05	kJ/mol	Joback Method
hfs	-280.80	kJ/mol	NIST Webbook
hfus	21.60	kJ/mol	Joback Method
hvap	58.23	kJ/mol	Joback Method
log10ws	-0.69		Crippen Method
logp	-1.154		Crippen Method
mcvol	63.900	ml/mol	McGowan Method
pc	7317.64	kPa	Joback Method
tb	550.69	K	Joback Method
tc	790.77	K	Joback Method
tf	430.49	K	Joback Method
vc	0.243	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	140.09	J/mol×K	550.69	Joback Method
cpg	145.38	J/mol×K	590.70	Joback Method
cpg	150.28	J/mol×K	630.72	Joback Method
cpg	154.80	J/mol×K	670.73	Joback Method
cpg	158.95	J/mol×K	710.74	Joback Method
cpg	162.73	J/mol×K	750.76	Joback Method
cpg	166.18	J/mol×K	790.77	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C556898&Units=SI

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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