(CH3)2NCOCN

Inchi: InChI=1S/C4H6N2O/c1-6(2)4(7)3-5/h1-2H3
InchiKey: DNRRZLQWEDPRRM-UHFFFAOYSA-N
Formula: C4H6N2O
SMILES: CN(C)C(=O)C#N
Mol. weight [g/mol]: 98.10
CAS: 16703-51-8

Physical Properties

Property code	Value	Unit	Source
affp	829.00	kJ/mol	NIST Webbook
basg	797.10	kJ/mol	NIST Webbook
gf	97.84	kJ/mol	Joback Method
hf	-6.06	kJ/mol	Joback Method
hfus	12.24	kJ/mol	Joback Method
hvap	43.77	kJ/mol	Joback Method
log10ws	0.29		Crippen Method
logp	-0.402		Crippen Method
mcvol	80.150	ml/mol	McGowan Method
pc	4077.71	kPa	Joback Method
tb	459.31	K	Joback Method
tc	661.40	K	Joback Method
tf	282.23	K	Joback Method
vc	0.309	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	154.83	J/mol×K	459.31	Joback Method
cpg	161.90	J/mol×K	492.99	Joback Method
cpg	168.58	J/mol×K	526.67	Joback Method
cpg	174.89	J/mol×K	560.36	Joback Method
cpg	180.84	J/mol×K	594.04	Joback Method
cpg	186.45	J/mol×K	627.72	Joback Method
cpg	191.72	J/mol×K	661.40	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16703518&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

affp:	Proton affinity
basg:	Gas basicity
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
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