

Formamide, N-(cyanomethyl)-

Inchi:	InChI=1S/C3H4N2O/c4-1-2-5-3-6/h3H,2H2,(H,5,6)
InchiKey:	HHENWUYAOCBSAE-UHFFFAOYSA-N
Formula:	C3H4N2O
SMILES:	N#CCNC=O
Mol. weight [g/mol]:	84.08
CAS:	5018-27-9

Physical Properties

Property code	Value	Unit	Source
gf	97.43	kJ/mol	Joback Method
hf	27.52	kJ/mol	Joback Method
hfus	12.42	kJ/mol	Joback Method
hvap	45.91	kJ/mol	Joback Method
log10ws	0.09		Crippen Method
logp	-0.744		Crippen Method
mcvol	66.060	ml/mol	McGowan Method
pc	4795.85	kPa	Joback Method
tb	468.95	K	Joback Method
tc	673.13	K	Joback Method
tf	283.22	K	Joback Method
vc	0.281	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	125.74	J/mol×K	468.95	Joback Method
cpg	130.75	J/mol×K	502.98	Joback Method
cpg	135.52	J/mol×K	537.01	Joback Method
cpg	140.03	J/mol×K	571.04	Joback Method
cpg	144.30	J/mol×K	605.07	Joback Method
cpg	148.33	J/mol×K	639.10	Joback Method
cpg	152.14	J/mol×K	673.13	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5018279&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

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

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