Acetamide, n-(cyanomethyl)-

Inchi: InChI=1S/C4H6N2O/c1-4(7)6-3-2-5/h3H2,1H3,(H,6,7)
InchiKey: LHWCUMYXUCPQSZ-UHFFFAOYSA-N
Formula: C4H6N2O
SMILES: CC(O)=NCC#N
Mol. weight [g/mol]: 98.10
CAS: 4814-80-6

Physical Properties

Property code	Value	Unit	Source
hf	-40.81	kJ/mol	Joback Method
hvap	55.05	kJ/mol	Joback Method
log10ws	-0.35		Crippen Method
logp	0.486		Crippen Method
mcvol	80.150	ml/mol	McGowan Method
pc	3740.80	kPa	Joback Method
tb	561.74	K	Joback Method
tc	765.82	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4814806&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

hf: Enthalpy of formation 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