Urea, 1-(2-cyanoethyl)-3-methyl-

Inchi: InChI=1S/C5H9N3O/c1-7-5(9)8-4-2-3-6/h2,4H2,1H3,(H2,7,8,9)
InchiKey: AXVHURAAIURJHZ-UHFFFAOYSA-N
Formula: C5H9N3O
SMILES: CN=C(O)NCCC#N
Mol. weight [g/mol]: 127.14
CAS: 7150-75-6

Physical Properties

Property code	Value	Unit	Source
hf	-7.98	kJ/mol	Joback Method
hvap	63.71	kJ/mol	Joback Method
log10ws	-0.45		Crippen Method
logp	0.033		Crippen Method
mcvol	104.220	ml/mol	McGowan Method
pc	3388.08	kPa	Joback Method
tb	634.79	K	Joback Method
tc	836.23	K	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7150756&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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