NCC(CH3)CO

Inchi: InChI=1S/C4H5NO/c1-4(6)2-3-5/h2H2,1H3
InchiKey: OPXYNEYEDHAXOM-UHFFFAOYSA-N
Formula: C4H3NO
SMILES: CC(=O)CC#N
Mol. weight [g/mol]: 81.07
CAS: 57681-10-4

Physical Properties

Property code	Value	Unit	Source
affp	798.00	kJ/mol	NIST Webbook
basg	765.50	kJ/mol	NIST Webbook
gf	-12.94	kJ/mol	Joback Method
hf	-73.59	kJ/mol	Joback Method
hfus	9.22	kJ/mol	Joback Method
hvap	41.72	kJ/mol	Joback Method
log10ws	-0.64		Crippen Method
logp	0.489		Crippen Method
mcvol	70.170	ml/mol	McGowan Method
pc	4088.15	kPa	Joback Method
tb	446.87	K	Joback Method
tc	651.57	K	Joback Method
tf	249.76	K	Joback Method
vc	0.291	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	126.58	J/mol×K	446.87	Joback Method
cpg	132.40	J/mol×K	480.99	Joback Method
cpg	137.95	J/mol×K	515.10	Joback Method
cpg	143.25	J/mol×K	549.22	Joback Method
cpg	148.29	J/mol×K	583.34	Joback Method
cpg	153.08	J/mol×K	617.45	Joback Method
cpg	157.62	J/mol×K	651.57	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C57681104&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

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