

Alpha-oxobutyronitrile

Inchi:	InChI=1S/C4H5NO/c1-2-4(6)3-5/h2H2,1H3
InchiKey:	JQLHQBWQAFDAGK-UHFFFAOYSA-N
Formula:	C4H5NO
SMILES:	CCC(=O)C#N
Mol. weight [g/mol]:	83.09
CAS:	4390-78-7

Physical Properties

Property code	Value	Unit	Source
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/molxK	446.87	Joback Method
cpg	132.40	J/molxK	480.99	Joback Method
cpg	137.95	J/molxK	515.10	Joback Method
cpg	143.25	J/molxK	549.22	Joback Method
cpg	148.29	J/molxK	583.34	Joback Method
cpg	153.08	J/molxK	617.45	Joback Method
cpg	157.62	J/molxK	651.57	Joback Method

Sources

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=C4390787&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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