

Butanenitrile, 4-oxo-

Other names:	Propanal, 3-cyano- «beta»-Cyanopropionaldehyde 3-formylpropiononitrile
Inchi:	InChI=1S/C4H5NO/c5-3-1-2-4-6/h4H,1-2H2
InchiKey:	CGFGIKNLZTZJDE-UHFFFAOYSA-N
Formula:	C4H5NO
SMILES:	N#CCCC=O
Mol. weight [g/mol]:	83.09
CAS:	3515-93-3

Physical Properties

Property code	Value	Unit	Source
chl	-2301.50 ± 1.50	kJ/mol	NIST Webbook
gf	16.46	kJ/mol	Joback Method
hf	-46.59	kJ/mol	Joback Method
hfl	12.80 ± 1.50	kJ/mol	NIST Webbook
hfus	9.91	kJ/mol	Joback Method
hvap	41.70	kJ/mol	Joback Method
log10ws	-0.64		Crippen Method
logp	0.489		Crippen Method
mcvol	70.170	ml/mol	McGowan Method
pc	4146.27	kPa	Joback Method
tb	441.66	K	Joback Method
tc	640.82	K	Joback Method
tf	241.83	K	Joback Method
vc	0.302	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	129.12	J/mol×K	441.66	Joback Method
cpg	134.70	J/mol×K	474.85	Joback Method
cpg	140.02	J/mol×K	508.05	Joback Method
cpg	145.09	J/mol×K	541.24	Joback Method

cpg	149.92	J/mol×K	574.43	Joback Method
cpg	154.51	J/mol×K	607.62	Joback Method
cpg	158.86	J/mol×K	640.82	Joback Method
cpl	195.90	J/mol×K	300.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3515933&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

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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

Latest version available from:

<https://www.chemeo.com/cid/40-765-8/Butanenitrile-4-oxo.pdf>

Generated by Cheméo on 2025-12-24 00:48:30.762197167 +0000 UTC m=+6285508.292237827.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.