

«alpha»-Cyanopropionaldehyde

Inchi:	InChI=1S/C4H5NO/c1-4(2-5)3-6/h3-4H,1H3
InchiKey:	IATHTLTVQXMDPC-UHFFFAOYSA-N
Formula:	C4H5NO
SMILES:	CC(C#N)C=O
Mol. weight [g/mol]:	83.09
CAS:	26692-50-2

Physical Properties

Property code	Value	Unit	Source
gf	14.02	kJ/mol	Joback Method
hf	-51.87	kJ/mol	Joback Method
hfus	6.39	kJ/mol	Joback Method
hvap	41.31	kJ/mol	Joback Method
log10ws	-0.40		Crippen Method
logp	0.345		Crippen Method
mcvol	70.170	ml/mol	McGowan Method
pc	4189.32	kPa	Joback Method
tb	441.22	K	Joback Method
tc	645.11	K	Joback Method
tf	226.83	K	Joback Method
vc	0.296	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	155.60	J/molxK	611.13	Joback Method
cpg	129.31	J/molxK	441.22	Joback Method
cpg	135.11	J/molxK	475.20	Joback Method
cpg	140.63	J/molxK	509.18	Joback Method
cpg	145.88	J/molxK	543.16	Joback Method
cpg	150.87	J/molxK	577.15	Joback Method
cpg	160.08	J/molxK	645.11	Joback Method
cpl	169.50	J/molxK	300.00	NIST Webbook

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=C26692502&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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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