

Acetone cyanohydrin

Other names:	«alpha»-Hydroxyisobutyronitrile Propanenitrile, 2-hydroxy-2-methyl- Lactonitrile, 2-methyl- 2-Cyano-2-propanol 2-Hydroxy-2-methylpropionitrile 2-Hydroxyisobutyronitrile 2-Methylactonitrile 2-Propanone, cyanohydrin 2-Cyanopropan-2-ol Acetoncianhidrinei Acetoncianidrina Acetoncyanhydrine Acetoncyanhydrin Acetone cyanhydrin Acetonecyanhydrine Acetonkyanhydrin Cyanhydrine d'acetone USAF RH-8 2-Cyano-2-hydroxypropane Rcra waste number P069 UN 1541 2-Hydroxy-2-methylpropanenitrile NSC 131093
Inchi:	InChI=1S/C4H7NO/c1-4(2,6)3-5/h6H,1-2H3
InchiKey:	MWFMGBPGAXYFAR-UHFFFAOYSA-N
Formula:	C4H7NO
SMILES:	CC(C)(O)C#N
Mol. weight [g/mol]:	85.10
CAS:	75-86-5

Physical Properties

Property code	Value	Unit	Source
chl	-2450.60 ± 0.80	kJ/mol	NIST Webbook
gf	-18.00	kJ/mol	Joback Method
hf	-121.99	kJ/mol	Joback Method
hfl	-120.90 ± 0.80	kJ/mol	NIST Webbook

hfus	4.30		kJ/mol	Joback Method
hvap	50.36		kJ/mol	Joback Method
ie	11.09		eV	NIST Webbook
log10ws	-0.74			Crippen Method
logp	0.281			Crippen Method
mcvol	74.470		ml/mol	McGowan Method
pc	4351.13		kPa	Joback Method
tb	481.95		K	Joback Method
tc	677.00		K	Joback Method
tf	251.90 ± 0.60		K	NIST Webbook
vc	0.293		m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	183.74	J/mol×K	644.49	Joback Method
cpg	155.39	J/mol×K	481.95	Joback Method
cpg	161.83	J/mol×K	514.46	Joback Method
cpg	167.86	J/mol×K	546.97	Joback Method
cpg	173.50	J/mol×K	579.47	Joback Method
cpg	178.79	J/mol×K	611.98	Joback Method
cpg	188.37	J/mol×K	677.00	Joback Method
hvapt	106.50	kJ/mol	374.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	355.20	K	3.10	NIST Webbook

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C75865&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas 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
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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