

Acetonitrile, hydroxy-

Other names:	Glycolonitrile Cyanomethanol Formaldehyde cyanohydrin Glycolic nitrile Glyconitrile Hydroxyacetonitrile Hydroxyactonitrile Hydroxymethylnitrile 2-Hydroxyacetonitrile HOCH ₂ CN USAF A-8565 2-Hydroxyethanenitrile Glykolonitril Hydroxymethylcyanid Acetonitrile, 2-hydroxy- NSC 1790 glycollonitrile
Inchi:	InChI=1S/C2H3NO/c3-1-2-4/h4H,2H2
InchiKey:	LTYRAPJYLUPLCI-UHFFFAOYSA-N
Formula:	C ₂ H ₃ NO
SMILES:	N#CCO
Mol. weight [g/mol]:	57.05
CAS:	107-16-4

Physical Properties

Property code	Value	Unit	Source
gf	-37.68	kJ/mol	Joback Method
hf	-71.96	kJ/mol	Joback Method
hfus	6.53	kJ/mol	Joback Method
hvap	47.20	kJ/mol	Joback Method
log10ws	0.21		Crippen Method
logp	-0.498		Crippen Method
mcvol	46.290	ml/mol	McGowan Method
pc	5544.32	kPa	Joback Method
tb	439.42	K	Joback Method
tc	626.60	K	Joback Method
tf	238.11	K	Joback Method

vc

0.193

m³/kmol

Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	79.88	J/mol×K	439.42	Joback Method
cpg	82.87	J/mol×K	470.62	Joback Method
cpg	85.74	J/mol×K	501.81	Joback Method
cpg	88.49	J/mol×K	533.01	Joback Method
cpg	91.13	J/mol×K	564.21	Joback Method
cpg	93.65	J/mol×K	595.41	Joback Method
cpg	96.07	J/mol×K	626.60	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	372.70	K	2.30	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C107164&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

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

h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
t_b:	Normal Boiling Point Temperature
t_{brp}:	Boiling point at reduced pressure
t_c:	Critical Temperature
t_f:	Normal melting (fusion) point
v_c:	Critical Volume

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