

GLYCOLONITRILE

Other names:	Glycolonitrile
	Cyanomethanol
	Formaldehyde cyanohydrin
	Glycolic nitrile
	Glyconitrile
	Hydroxyacetonitrile
	Hydroxyactonitrile
	Hydroxymethylnitrile
	2-Hydroxyacetonitrile
	HOCH2CN
	USAF A-8565
	2-Hydroxyethanenitrile
	Glykolonitril
	Hydroxymethylkyanid
	Acetonitrile, 2-hydroxy-
	NSC 1790
	glycollonitrile
Inchi:	InChI=1S/C2H3NO/c3-1-2-4/h4H,2H2
InchiKey:	LTYRAPJYLUPLCI-UHFFFAOYSA-N
Formula:	C2H3NO
SMILES:	N#CCO
Mol. weight [g/mol]:	57.05

Physical Properties

Property code	Value	Unit	Source
af	0.5822		Cheméo Relay (1.0)
gf	-37.68	kJ/mol	Joback Method
hf	-71.77	kJ/mol	Cheméo Relay (1.0)
hfus	6.53	kJ/mol	Joback Method
hvap	56.02	kJ/mol	Cheméo Relay (1.0)
ie	11.65	eV	Cheméo Relay (1.0)
logp	-0.498		Crippen Method
mcvol	46.290	ml/mol	McGowan Method
pc	5544.32	kPa	Joback Method
tb	453.72	K	Cheméo Relay (1.0)
tc	686.45	K	Cheméo Relay (1.0)
tf	230.91	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C107164&Units=SI>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

McGowan Method:

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

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

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

Legend

af: Acentric Factor

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
hvac:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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

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