

CH2NO2

Inchi:	InChI=1S/CH2NO2/c1-2(3)4/h1H2
InchiKey:	VUHWIBLKRDNZSP-UHFFFAOYSA-N
Formula:	CH2NO2
SMILES:	[CH2][N+](=O)[O-]
Mol. weight [g/mol]:	60.03
CAS:	16787-85-2

Physical Properties

Property code	Value	Unit	Source
gf	45.47	kJ/mol	Joback Method
hf	-18.92	kJ/mol	Joback Method
hfus	11.39	kJ/mol	Joback Method
hvap	34.26	kJ/mol	Joback Method
log10ws	-0.43		Crippen Method
logp	0.055		Crippen Method
mcvol	40.220	ml/mol	McGowan Method
pc	6318.86	kPa	Joback Method
tb	373.42	K	Joback Method
tc	583.02	K	Joback Method
tf	261.01	K	Joback Method
vc	0.165	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	62.16	J/molxK	373.42	Joback Method
cpg	66.11	J/molxK	408.35	Joback Method
cpg	69.68	J/molxK	443.29	Joback Method
cpg	72.89	J/molxK	478.22	Joback Method
cpg	75.78	J/molxK	513.15	Joback Method
cpg	78.39	J/molxK	548.09	Joback Method
cpg	80.74	J/molxK	583.02	Joback Method

Sources

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=C16787852&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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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