2-(Hydroxymethyl)but-2-enenitrile

Inchi: InChI=1S/C5H7NO/c1-2-5(3-6)4-7/h2,7H,4H2,1H3/b5-2-
InchiKey: KVPZUICDNYJQMU-DJWKRKHSSA-N
Formula: C5H7NO
SMILES: CC=C(C#N)CO
Mol. weight [g/mol]: 97.12
CAS: 139443-52-0

Physical Properties

Property code	Value	Unit	Source
gf	59.25	kJ/mol	Joback Method
hf	-26.45	kJ/mol	Joback Method
hfus	13.19	kJ/mol	Joback Method
hvap	53.92	kJ/mol	Joback Method
log10ws	-0.90		Crippen Method
logp	0.449		Crippen Method
mcvol	84.260	ml/mol	McGowan Method
pc	4036.37	kPa	Joback Method
rinpol	1006.90		NIST Webbook
rinpol	1006.90		NIST Webbook
tb	512.10	K	Joback Method
tc	705.29	K	Joback Method
tf	252.88	K	Joback Method
vc	0.342	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	172.23	J/mol×K	512.10	Joback Method
cpg	178.66	J/mol×K	544.30	Joback Method
cpg	184.73	J/mol×K	576.50	Joback Method
cpg	190.48	J/mol×K	608.69	Joback Method
cpg	195.91	J/mol×K	640.89	Joback Method
cpg	201.06	J/mol×K	673.09	Joback Method
cpg	205.94	J/mol×K	705.29	Joback Method

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=C139443520&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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