4-(methylthio)butenenitrile

Inchi: InChI=1S/C5H7NS/c1-7-5-3-2-4-6/h2-3H,5H2,1H3/b3-2+
InchiKey: CGSLHZQOUDWXEN-NSCUHMNNSA-N
Formula: C5H7NS
SMILES: CSCC=CC#N
Mol. weight [g/mol]: 113.18

Physical Properties

Property code	Value	Unit	Source
gf	237.74	kJ/mol	Joback Method
hf	177.44	kJ/mol	Joback Method
hfus	14.54	kJ/mol	Joback Method
hvap	43.98	kJ/mol	Joback Method
log10ws	-1.52		Crippen Method
logp	1.429		Crippen Method
mcvol	94.740	ml/mol	McGowan Method
pc	3655.35	kPa	Joback Method
rinpol	1091.00		NIST Webbook
rinpol	1091.00		NIST Webbook
tb	488.82	K	Joback Method
tc	712.96	K	Joback Method
tf	240.42	K	Joback Method
vc	0.376	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	174.88	J/mol×K	488.82	Joback Method
cpg	182.77	J/mol×K	526.18	Joback Method
cpg	190.20	J/mol×K	563.53	Joback Method
cpg	197.19	J/mol×K	600.89	Joback Method
cpg	203.77	J/mol×K	638.25	Joback Method
cpg	209.94	J/mol×K	675.61	Joback Method
cpg	215.74	J/mol×K	712.96	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=R239239&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume