4-(Methylsulfinyl)butanenitrile

Inchi: InChI=1S/C5H9NOS/c1-8(7)5-3-2-4-6/h2-3,5H2,1H3
InchiKey: XCDBAGVWCGHEFB-UHFFFAOYSA-N
Formula: C5H9NOS
SMILES: CS(=O)CCCC#N
Mol. weight [g/mol]: 131.20
CAS: 61121-65-1

Physical Properties

Property code	Value	Unit	Source
gf	-93.31	kJ/mol	Joback Method
hf	-187.39	kJ/mol	Joback Method
hfus	17.97	kJ/mol	Joback Method
hvap	49.93	kJ/mol	Joback Method
log10ws	-0.42		Crippen Method
logp	0.669		Crippen Method
mcvol	104.910	ml/mol	McGowan Method
pc	3731.66	kPa	Joback Method
rinpol	1372.90		NIST Webbook
rinpol	1372.90		NIST Webbook
tb	474.16	K	Joback Method
tc	673.54	K	Joback Method
tf	247.58	K	Joback Method
vc	0.431	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	207.22	J/mol×K	474.16	Joback Method
cpg	215.99	J/mol×K	507.39	Joback Method
cpg	224.38	J/mol×K	540.62	Joback Method
cpg	232.40	J/mol×K	573.85	Joback Method
cpg	240.04	J/mol×K	607.08	Joback Method
cpg	247.31	J/mol×K	640.31	Joback Method
cpg	254.20	J/mol×K	673.54	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C61121651&Units=SI

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