8-Methylthiooctanonitrile

Inchi: InChI=1S/C9H17NS/c1-11-9-7-5-3-2-4-6-8-10/h2-7,9H2,1H3
InchiKey: BWZCPICNIWWLFX-UHFFFAOYSA-N
Formula: C9H17NS
SMILES: CSCCCCCCCC#N
Mol. weight [g/mol]: 171.30
CAS: 58214-93-0

Physical Properties

Property code	Value	Unit	Source
gf	191.20	kJ/mol	Joback Method
hf	-22.34	kJ/mol	Joback Method
hfus	24.70	kJ/mol	Joback Method
hvap	52.92	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	3.214		Crippen Method
mcvol	155.400	ml/mol	McGowan Method
pc	2289.32	kPa	Joback Method
rinpol	1533.50		NIST Webbook
rinpol	1533.50		NIST Webbook
tb	576.18	K	Joback Method
tc	777.15	K	Joback Method
tf	290.58	K	Joback Method
vc	0.620	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	366.20	J/mol×K	576.18	Joback Method
cpg	379.11	J/mol×K	609.68	Joback Method
cpg	391.39	J/mol×K	643.17	Joback Method
cpg	403.06	J/mol×K	676.67	Joback Method
cpg	414.12	J/mol×K	710.16	Joback Method
cpg	424.59	J/mol×K	743.66	Joback Method
cpg	434.49	J/mol×K	777.15	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=C58214930&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