1-Cyano-2,3-epithiopropane

Other names: Thiirane-2-acetonitrile
Inchi: InChI=1S/C4H5NS/c5-2-1-4-3-6-4/h4H,1,3H2
InchiKey: BKIZJNMVTRYGSW-UHFFFAOYSA-N
Formula: C4H5NS
SMILES: N#CCC1CS1
Mol. weight [g/mol]: 99.15
CAS: 58130-93-1

Physical Properties

Property code	Value	Unit	Source
gf	216.59	kJ/mol	Joback Method
hf	157.05	kJ/mol	Joback Method
hfus	9.41	kJ/mol	Joback Method
hvap	40.70	kJ/mol	Joback Method
log10ws	-1.25		Crippen Method
logp	1.015		Crippen Method
mcvol	74.090	ml/mol	McGowan Method
pc	4426.72	kPa	Joback Method
rinpol	874.00		NIST Webbook
rinpol	874.00		NIST Webbook
tb	447.57	K	Joback Method
tc	673.26	K	Joback Method
tf	301.22	K	Joback Method
vc	0.288	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	136.34	J/mol×K	447.57	Joback Method
cpg	143.84	J/mol×K	485.18	Joback Method
cpg	150.77	J/mol×K	522.80	Joback Method
cpg	157.19	J/mol×K	560.41	Joback Method
cpg	163.12	J/mol×K	598.03	Joback Method
cpg	168.61	J/mol×K	635.64	Joback Method

cpg	173.72	J/mol×K	673.26	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=C58130931&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