

1-cyano-3,4-epithiobutane

Other names:	3,4-Epoxythiobutyl cyanide
Inchi:	InChI=1S/C5H7NS/c6-3-1-2-5-4-7-5/h5H,1-2,4H2
InchiKey:	ZAGXORSINWAUSP-UHFFFAOYSA-N
Formula:	C5H7NS
SMILES:	N#CCCC1CS1
Mol. weight [g/mol]:	113.18
CAS:	54096-45-6

Physical Properties

Property code	Value	Unit	Source
gf	225.01	kJ/mol	Joback Method
hf	136.41	kJ/mol	Joback Method
hfus	12.00	kJ/mol	Joback Method
hvap	42.93	kJ/mol	Joback Method
log10ws	-1.67		Crippen Method
logp	1.406		Crippen Method
mcvol	88.180	ml/mol	McGowan Method
pc	3911.14	kPa	Joback Method
rinpol	1124.00		NIST Webbook
rinpol	1122.50		NIST Webbook
rinpol	1122.50		NIST Webbook
rinpol	1075.00		NIST Webbook
rinpol	1086.00		NIST Webbook
rinpol	1086.00		NIST Webbook
tb	470.45	K	Joback Method
tc	692.69	K	Joback Method
tf	312.49	K	Joback Method
vc	0.344	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	173.95	J/molxK	470.45	Joback Method
cpg	182.86	J/molxK	507.49	Joback Method

cpg	191.15	J/mol×K	544.53	Joback Method
cpg	198.86	J/mol×K	581.57	Joback Method
cpg	206.03	J/mol×K	618.61	Joback Method
cpg	212.72	J/mol×K	655.65	Joback Method
cpg	218.97	J/mol×K	692.69	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=C54096456&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	McGowan's characteristic volume
pc:	Critical Pressure
r inpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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