

(Z)-1-Methyl-3-(prop-1-en-1-yl)trisulfane

Inchi:	InChI=1S/C4H8S3/c1-3-4-6-7-5-2/h3-4H,1-2H3/b4-3-
InchiKey:	WPRUFZZPIFLBDG-ARJAWSKDSA-N
Formula:	C4H8S3
SMILES:	CC=CSSSC
Mol. weight [g/mol]:	152.30
CAS:	23838-24-6

Physical Properties

Property code	Value	Unit	Source
gf	162.38	kJ/mol	Joback Method
hf	116.94	kJ/mol	Joback Method
hfus	18.71	kJ/mol	Joback Method
hvap	44.91	kJ/mol	Joback Method
log10ws	-3.48		Crippen Method
logp	3.179		Crippen Method
mcvol	111.970	ml/mol	McGowan Method
pc	4450.38	kPa	Joback Method
rinpol	1163.70		NIST Webbook
tb	501.42	K	Joback Method
tc	756.84	K	Joback Method
tf	232.96	K	Joback Method
vc	0.402	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	198.58	J/mol×K	501.42	Joback Method
cpg	208.10	J/mol×K	543.99	Joback Method
cpg	217.06	J/mol×K	586.56	Joback Method
cpg	225.46	J/mol×K	629.13	Joback Method
cpg	233.29	J/mol×K	671.70	Joback Method
cpg	240.57	J/mol×K	714.27	Joback Method
cpg	247.28	J/mol×K	756.84	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C23838246&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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