

(E)-1,3-Bis-(methylthio)propene

Inchi:

InChI=1S/C5H10S2/c1-6-4-3-5-7-2/h3-4H,5H2,1-2H3/b4-3+

InchiKey:

HRYLOXZUQKTDRD-ONEGZZNKSA-N

Formula:

C5H10S2

SMILES:

CSC=CCSC

Mol. weight [g/mol]:

134.26

Physical Properties

Property code	Value	Unit	Source
gf	137.68	kJ/mol	Joback Method
hf	54.43	kJ/mol	Joback Method
hfus	17.17	kJ/mol	Joback Method
hvap	40.32	kJ/mol	Joback Method
log10ws	-2.03		Crippen Method
logp	2.226		Crippen Method
mcvol	109.710	ml/mol	McGowan Method
pc	3848.31	kPa	Joback Method
ripol	1654.00		NIST Webbook
ripol	1654.00		NIST Webbook
tb	455.52	K	Joback Method
tc	681.95	K	Joback Method
tf	209.83	K	Joback Method
vc	0.404	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	197.10	J/mol×K	455.52	Joback Method
cpg	207.53	J/mol×K	493.26	Joback Method
cpg	217.41	J/mol×K	531.00	Joback Method
cpg	226.76	J/mol×K	568.74	Joback Method
cpg	235.58	J/mol×K	606.47	Joback Method
cpg	243.90	J/mol×K	644.21	Joback Method
cpg	251.73	J/mol×K	681.95	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=R319781&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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