

bis(mercaptomethyl) sulfide

Inchi:	InChI=1S/C2H6S3/c3-1-5-2-4/h3-4H,1-2H2
InchiKey:	WTSBJMAOQNCZBF-UHFFFAOYSA-N
Formula:	C2H6S3
SMILES:	SCSCS
Mol. weight [g/mol]:	126.26

Physical Properties

Property code	Value	Unit	Source
gf	57.86	kJ/mol	Joback Method
hf	34.22	kJ/mol	Joback Method
hfus	13.15	kJ/mol	Joback Method
hvap	40.34	kJ/mol	Joback Method
log10ws	-1.68		Crippen Method
logp	1.494		Crippen Method
mcvol	88.090	ml/mol	McGowan Method
pc	6249.12	kPa	Joback Method
rinpola	960.00		NIST Webbook
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tb	439.66	K	Joback Method
tc	692.58	K	Joback Method
tf	219.62	K	Joback Method
vc	0.309	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	139.55	J/mol×K	439.66	Joback Method
cpg	146.21	J/mol×K	481.81	Joback Method
cpg	152.52	J/mol×K	523.97	Joback Method
cpg	158.49	J/mol×K	566.12	Joback Method
cpg	164.13	J/mol×K	608.27	Joback Method
cpg	169.42	J/mol×K	650.42	Joback Method
cpg	174.36	J/mol×K	692.58	Joback Method

Sources

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=R210496&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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