

Dithiomethane, methyl

Inchi:

InChI=1S/C2H6S2/c1-4-2-3/h3H,2H2,1H3

InchiKey:

IXBUFAUQDFHNGI-UHFFFAOYSA-N

Formula:

C2H6S2

SMILES:

CSCS

Mol. weight [g/mol]:

94.20

Physical Properties

Property code	Value	Unit	Source
gf	28.47	kJ/mol	Joback Method
hf	-4.26	kJ/mol	Joback Method
hfus	9.11	kJ/mol	Joback Method
hvap	33.60	kJ/mol	Joback Method
log10ws	-1.11		Crippen Method
logp	1.237		Crippen Method
mcvol	71.740	ml/mol	McGowan Method
pc	5661.74	kPa	Joback Method
rinpol	723.00		NIST Webbook
rinpol	723.00		NIST Webbook
rinpol	725.00		NIST Webbook
tb	376.80	K	Joback Method
tc	599.98	K	Joback Method
tf	183.16	K	Joback Method
vc	0.256	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	106.72	J/mol×K	376.80	Joback Method
cpg	112.60	J/mol×K	414.00	Joback Method
cpg	118.25	J/mol×K	451.19	Joback Method
cpg	123.69	J/mol×K	488.39	Joback Method
cpg	128.90	J/mol×K	525.59	Joback Method
cpg	133.89	J/mol×K	562.79	Joback Method
cpg	138.64	J/mol×K	599.98	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=R62350&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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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