

S-methyl 2-methylpropanethioate

Other names:	S-Methyl thio-2-methylpropanoate
Inchi:	InChI=1S/C5H10OS/c1-4(2)5(6)7-3/h4H,1-3H3
InchiKey:	JODNYDRGCYHKRC-UHFFFAOYSA-N
Formula:	C5H10OS
SMILES:	CSC(=O)C(C)C
Mol. weight [g/mol]:	118.20

Physical Properties

Property code	Value	Unit	Source
af	0.3069		Cheméo Relay (1.0)
hf	-252.63	kJ/mol	Cheméo Relay (1.0)
hfus	10.91	kJ/mol	Joback Method
hvap	41.24	kJ/mol	Cheméo Relay (1.0)
ie	9.12	eV	Cheméo Relay (1.0)
log10ws	-1.26		Cheméo Relay (1.0)
logp	1.532		Crippen Method
mcvol	99.230	ml/mol	McGowan Method
pc	3857.88	kPa	Joback Method
ripol	1141.00		NIST Webbook
ripol	1141.00		NIST Webbook
ripol	1140.00		NIST Webbook
tb	398.69	K	Cheméo Relay (1.0)
tc	583.85	K	Cheméo Relay (1.0)
tf	228.59	K	Cheméo Relay (1.0)
vc	0.343	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	184.66	J/mol×K	436.01	Joback Method
cpg	194.48	J/mol×K	470.68	Joback Method
cpg	203.89	J/mol×K	505.35	Joback Method
cpg	212.87	J/mol×K	540.02	Joback Method
cpg	221.43	J/mol×K	574.69	Joback Method

cpg	229.58	J/mol×K	609.36	Joback Method
cpg	237.31	J/mol×K	644.03	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C42075423&Units=SI>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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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