2,3,5-TRITHIAHEXANE

Other names:	Methyl methylthiomethyl disulfide
	2,4,5-Trithiahexane
	2,3,5-Trithiahexane
	Methane, (methyldithio)(methylthio)-
	Methyl (methylthio)methyl disulphide
	1-(methylthio)dimethyl disulfide
Inchi:	InChI=1S/C3H8S3/c1-4-3-6-5-2/h3H2,1-2H3
InchiKey:	MYIOBINSHMEDEY-UHFFFAOYSA-N
Formula:	C3H8S3
SMILES:	CSCSSC
Mol. weight [g/mol]:	140.30

Physical Properties

Property code	Value	Unit	Source
hf	-1.19	kJ/mol	Cheméo Relay (1.0)
hfus	15.92	kJ/mol	Joback Method
ie	8.49	eV	Cheméo Relay (1.0)
logp	2.318		Crippen Method
mcvol	102.180	ml/mol	McGowan Method
rinpol	1154.00		NIST Webbook
rinpol	1110.00		NIST Webbook
rinpol	1143.00		NIST Webbook
rinpol	1144.00		NIST Webbook
rinpol	1099.00		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1134.10		NIST Webbook
rinpol	1109.00		NIST Webbook
rinpol	1104.00		NIST Webbook
rinpol	1139.00		NIST Webbook
rinpol	1147.00		NIST Webbook
rinpol	1143.00		NIST Webbook
rinpol	1144.00		NIST Webbook
rinpol	1147.00		NIST Webbook
rinpol	1134.10		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1106.00		NIST Webbook
rinpol	1097.00		NIST Webbook

rinpol	1146.00		NIST Webbook
rinpol	1094.00		NIST Webbook
rinpol	1099.00		NIST Webbook
rinpol	1139.00		NIST Webbook
ripol	1650.00		NIST Webbook
ripol	1650.00		NIST Webbook
ripol	1662.00		NIST Webbook
ripol	1705.50		NIST Webbook
ripol	1630.00		NIST Webbook
ripol	1632.00		NIST Webbook
ripol	1666.00		NIST Webbook
ripol	1630.00		NIST Webbook
ripol	1705.50		NIST Webbook
tb	471.35	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	177.54	J/mol×K	474.38	Joback Method
cpg	186.23	J/mol×K	515.65	Joback Method
cpg	194.55	J/mol×K	556.92	Joback Method
cpg	202.47	J/mol×K	598.18	Joback Method
cpg	209.97	J/mol×K	639.45	Joback Method
cpg	217.02	J/mol×K	680.72	Joback Method
cpg	223.61	J/mol×K	721.99	Joback Method

Sources

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C42474442&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/ci990307l

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature