

Methyl propyl trisulfide

Other names:	Trisulfide, methyl propyl Methyl propyl trisulphide Methyl n-propyl trisulfide
Inchi:	InChI=1S/C4H10S3/c1-3-4-6-7-5-2/h3-4H2,1-2H3
InchiKey:	ZOYASYRPGHCQHW-UHFFFAOYSA-N
Formula:	C4H10S3
SMILES:	CCCCSSSC
Mol. weight [g/mol]:	154.32
CAS:	17619-36-2

Physical Properties

Property code	Value	Unit	Source
gf	82.16	kJ/mol	Joback Method
hf	-0.28	kJ/mol	Joback Method
hfus	18.51	kJ/mol	Joback Method
hvap	44.95	kJ/mol	Joback Method
log10ws	-3.13		Crippen Method
logp	3.056		Crippen Method
mcvol	116.270	ml/mol	McGowan Method
pc	4156.97	kPa	Joback Method
rinpol	1137.00		NIST Webbook
rinpol	1150.00		NIST Webbook
rinpol	1137.00		NIST Webbook
rinpol	1097.00		NIST Webbook
rinpol	1143.00		NIST Webbook
rinpol	1116.00		NIST Webbook
rinpol	1168.00		NIST Webbook
rinpol	1132.00		NIST Webbook
rinpol	1154.20		NIST Webbook
rinpol	1132.00		NIST Webbook
rinpol	1134.00		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1118.10		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1134.00		NIST Webbook
rinpol	1134.00		NIST Webbook
rinpol	1146.00		NIST Webbook

rinpol	1137.00		NIST Webbook
ripol	1539.00		NIST Webbook
ripol	1523.00		NIST Webbook
ripol	1576.00		NIST Webbook
ripol	1519.00		NIST Webbook
ripol	1531.00		NIST Webbook
ripol	1529.00		NIST Webbook
tb	497.26	K	Joback Method
tc	740.19	K	Joback Method
tf	238.04	K	Joback Method
vc	0.421	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	216.75	J/mol×K	497.26	Joback Method
cpg	227.03	J/mol×K	537.75	Joback Method
cpg	236.83	J/mol×K	578.24	Joback Method
cpg	246.12	J/mol×K	618.73	Joback Method
cpg	254.89	J/mol×K	659.22	Joback Method
cpg	263.12	J/mol×K	699.70	Joback Method
cpg	270.79	J/mol×K	740.19	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C17619362&Units=SI

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

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