1-Methyl-3-propyltrisulfane

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: CCCSSSC
Mol. weight [g/mol]: 154.33

Physical Properties

Property code	Value	Unit	Source
hf	-32.13	kJ/mol	Cheméo Relay (1.0)
hfus	18.51	kJ/mol	Joback Method
hvap	55.44	kJ/mol	Cheméo Relay (1.0)
ie	8.43	eV	Cheméo Relay (1.0)
logp	3.056		Crippen Method
mcvol	116.270	ml/mol	McGowan Method
rinpol	1134.00		NIST Webbook
rinpol	1132.00		NIST Webbook
rinpol	1137.00		NIST Webbook
rinpol	1134.00		NIST Webbook
rinpol	1137.00		NIST Webbook
rinpol	1150.00		NIST Webbook
rinpol	1146.00		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1118.10		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1097.00		NIST Webbook
rinpol	1134.00		NIST Webbook
rinpol	1137.00		NIST Webbook
rinpol	1143.00		NIST Webbook
rinpol	1154.20		NIST Webbook
rinpol	1132.00		NIST Webbook
rinpol	1168.00		NIST Webbook
rinpol	1116.00		NIST Webbook
ripol	1519.00		NIST Webbook
ripol	1576.00		NIST Webbook

ripol	1523.00		NIST Webbook
ripol	1539.00		NIST Webbook
ripol	1529.00		NIST Webbook
ripol	1531.00		NIST Webbook
tb	481.92	K	Cheméo Relay (1.0)
tc	713.27	K	Cheméo Relay (1.0)
tf	228.64	K	Cheméo Relay (1.0)

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
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C17619362&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

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
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point