2,3,4-trithiahexane

Other names: Methyl ethyl trisulfide
ethyl methyl trisulfide
Inchi: InChI=1S/C3H8S3/c1-3-5-6-4-2/h3H2,1-2H3
InchiKey: XEKUTWIJPKGAQT-UHFFFAOYSA-N
Formula: C3H8S3
SMILES: CCSSSC
Mol. weight [g/mol]: 140.29

Physical Properties

Property code	Value	Unit	Source
gf	73.74	kJ/mol	Joback Method
hf	20.36	kJ/mol	Joback Method
hfus	15.92	kJ/mol	Joback Method
hvap	42.72	kJ/mol	Joback Method
log10ws	-2.71		Crippen Method
logp	2.666		Crippen Method
mcvol	102.180	ml/mol	McGowan Method
pc	4723.61	kPa	Joback Method
rinpol	1044.00		NIST Webbook
rinpol	1030.00		NIST Webbook
rinpol	1054.00		NIST Webbook
rinpol	1054.00		NIST Webbook
rinpol	1082.00		NIST Webbook
rinpol	1030.00		NIST Webbook
tb	474.38	K	Joback Method
tc	721.99	K	Joback Method
tf	226.77	K	Joback Method
vc	0.365	m3/kmol	Joback Method

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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R53440&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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