2,3,4,5-tetrathiaheptane

Other names: Methyl ethyl tetrasulfide
Inchi: InChI=1S/C3H8S4/c1-3-5-7-6-4-2/h3H2,1-2H3
InchiKey: AEWINZMMMZGEST-UHFFFAOYSA-N
Formula: C3H8S4
SMILES: CCSSSSC
Mol. weight [g/mol]: 172.36

Physical Properties

Property code	Value	Unit	Source
gf	106.86	kJ/mol	Joback Method
hf	62.23	kJ/mol	Joback Method
hfus	20.05	kJ/mol	Joback Method
hvap	49.54	kJ/mol	Joback Method
log10ws	-3.58		Crippen Method
logp	3.314		Crippen Method
mcvol	118.530	ml/mol	McGowan Method
pc	4835.95	kPa	Joback Method
rinpol	1280.00		NIST Webbook
rinpol	1278.00		NIST Webbook
rinpol	1321.00		NIST Webbook
tb	543.16	K	Joback Method
tc	815.04	K	Joback Method
tf	261.17	K	Joback Method
vc	0.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.81	J/mol×K	543.16	Joback Method
cpg	225.24	J/mol×K	588.47	Joback Method
cpg	234.13	J/mol×K	633.79	Joback Method
cpg	242.44	J/mol×K	679.10	Joback Method
cpg	250.12	J/mol×K	724.42	Joback Method
cpg	257.12	J/mol×K	769.73	Joback Method

cpg	263.40	J/mol×K	815.04	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=R53436&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume