2-methyl-3,4,5-trithiaheptane

Inchi: InChI=1S/C5H12S3/c1-4-6-8-7-5(2)3/h5H,4H2,1-3H3
InchiKey: PWJZVOZMBUCSOV-UHFFFAOYSA-N
Formula: C5H12S3
SMILES: CCSSSC(C)C
Mol. weight [g/mol]: 168.34

Physical Properties

Property code	Value	Unit	Source
gf	88.14	kJ/mol	Joback Method
hf	-26.20	kJ/mol	Joback Method
hfus	17.57	kJ/mol	Joback Method
hvap	46.79	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	3.444		Crippen Method
mcvol	130.360	ml/mol	McGowan Method
pc	3722.56	kPa	Joback Method
rinpol	1199.00		NIST Webbook
rinpol	1199.00		NIST Webbook
tb	519.70	K	Joback Method
tc	763.71	K	Joback Method
tf	234.31	K	Joback Method
vc	0.471	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.40	J/mol×K	519.70	Joback Method
cpg	270.44	J/mol×K	560.37	Joback Method
cpg	281.85	J/mol×K	601.04	Joback Method
cpg	292.62	J/mol×K	641.70	Joback Method
cpg	302.74	J/mol×K	682.37	Joback Method
cpg	312.18	J/mol×K	723.04	Joback Method
cpg	320.94	J/mol×K	763.71	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R156020&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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