Methyl 2-propenyl pentasulfide

Inchi: InChI=1S/C4H8S5/c1-3-4-6-8-9-7-5-2/h3H,1,4H2,2H3
InchiKey: BFVOYECMMKLFQJ-UHFFFAOYSA-N
Formula: C4H8S5
SMILES: C=CCSSSSSC
Mol. weight [g/mol]: 216.43

Physical Properties

Property code	Value	Unit	Source
gf	236.24	kJ/mol	Joback Method
hf	208.89	kJ/mol	Joback Method
hfus	25.49	kJ/mol	Joback Method
hvap	57.91	kJ/mol	Joback Method
log10ws	-4.73		Crippen Method
logp	4.128		Crippen Method
mcvol	144.670	ml/mol	McGowan Method
pc	4596.38	kPa	Joback Method
rinpol	1535.00		NIST Webbook
rinpol	1572.00		NIST Webbook
rinpol	1567.00		NIST Webbook
tb	631.50	K	Joback Method
tc	924.60	K	Joback Method
tf	305.08	K	Joback Method
vc	0.510	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	278.83	J/mol×K	631.50	Joback Method
cpg	288.92	J/mol×K	680.35	Joback Method
cpg	298.11	J/mol×K	729.20	Joback Method
cpg	306.34	J/mol×K	778.05	Joback Method
cpg	313.57	J/mol×K	826.90	Joback Method
cpg	319.72	J/mol×K	875.75	Joback Method
cpg	324.74	J/mol×K	924.60	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R53404&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