Methyl propenyl pentasulfide

Inchi: InChI=1S/C4H8S5/c1-3-4-6-8-9-7-5-2/h3-4H,1-2H3/b4-3+
InchiKey: DKONGALMQJOVEV-ONEGZZNKSA-N
Formula: C4H8S5
SMILES: CC=CSSSSSC
Mol. weight [g/mol]: 216.43

Physical Properties

Property code	Value	Unit	Source
gf	228.62	kJ/mol	Joback Method
hf	200.68	kJ/mol	Joback Method
hfus	26.97	kJ/mol	Joback Method
hvap	58.54	kJ/mol	Joback Method
log10ws	-5.23		Crippen Method
logp	4.476		Crippen Method
mcvol	144.670	ml/mol	McGowan Method
pc	4659.34	kPa	Joback Method
rinpol	1588.00		NIST Webbook
rinpol	1588.00		NIST Webbook
tb	638.98	K	Joback Method
tc	938.79	K	Joback Method
tf	301.76	K	Joback Method
vc	0.509	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.78	J/mol×K	638.98	Joback Method
cpg	287.89	J/mol×K	688.95	Joback Method
cpg	297.06	J/mol×K	738.92	Joback Method
cpg	305.24	J/mol×K	788.88	Joback Method
cpg	312.41	J/mol×K	838.85	Joback Method
cpg	318.51	J/mol×K	888.82	Joback Method
cpg	323.50	J/mol×K	938.79	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R410750&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