Bis(1-methyl thio)propyl disulfide

Inchi: InChI=1S/C8H18S4/c1-5-7(9-3)11-12-8(6-2)10-4/h7-8H,5-6H2,1-4H3
InchiKey: LHVBQVQKDUZOIJ-UHFFFAOYSA-N
Formula: C8H18S4
SMILES: CCC(SC)SSC(CC)SC
Mol. weight [g/mol]: 242.49

Physical Properties

Property code	Value	Unit	Source
gf	144.08	kJ/mol	Joback Method
hf	-51.53	kJ/mol	Joback Method
hfus	25.95	kJ/mol	Joback Method
hvap	59.89	kJ/mol	Joback Method
log10ws	-4.91		Crippen Method
logp	4.566		Crippen Method
mcvol	188.980	ml/mol	McGowan Method
pc	2764.26	kPa	Joback Method
rinpol	1426.00		NIST Webbook
tb	656.68	K	Joback Method
tc	909.52	K	Joback Method
tf	287.52	K	Joback Method
vc	0.688	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	446.70	J/mol×K	656.68	Joback Method
cpg	462.17	J/mol×K	698.82	Joback Method
cpg	476.53	J/mol×K	740.96	Joback Method
cpg	489.75	J/mol×K	783.10	Joback Method
cpg	501.84	J/mol×K	825.24	Joback Method
cpg	512.76	J/mol×K	867.38	Joback Method
cpg	522.53	J/mol×K	909.52	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R415884&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