2,5,6-trimethyl-3,4-dithiaheptane

Inchi: InChI=1S/C8H18S2/c1-6(2)8(5)10-9-7(3)4/h6-8H,1-5H3
InchiKey: XVUIFQKOTMJJIU-UHFFFAOYSA-N
Formula: C8H18S2
SMILES: CC(C)SSC(C)C(C)C
Mol. weight [g/mol]: 178.36

Physical Properties

Property code	Value	Unit	Source
gf	75.40	kJ/mol	Joback Method
hf	-140.55	kJ/mol	Joback Method
hfus	14.17	kJ/mol	Joback Method
hvap	45.87	kJ/mol	Joback Method
log10ws	-3.91		Crippen Method
logp	3.821		Crippen Method
mcvol	156.280	ml/mol	McGowan Method
pc	2690.21	kPa	Joback Method
rinpol	1191.00		NIST Webbook
tb	518.68	K	Joback Method
tc	738.98	K	Joback Method
tf	203.72	K	Joback Method
vc	0.574	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	341.53	J/mol×K	518.68	Joback Method
cpg	357.25	J/mol×K	555.40	Joback Method
cpg	372.18	J/mol×K	592.11	Joback Method
cpg	386.31	J/mol×K	628.83	Joback Method
cpg	399.67	J/mol×K	665.55	Joback Method
cpg	412.26	J/mol×K	702.26	Joback Method
cpg	424.08	J/mol×K	738.98	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=R155710&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