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

Inchi: InChI=1S/C9H20S2/c1-7(2)10-9(5,6)11-8(3)4/h7-8H,1-6H3
InchiKey: XDSAVWGEUYYYGM-UHFFFAOYSA-N
Formula: C9H20S2
SMILES: CC(C)SC(C)(C)SC(C)C
Mol. weight [g/mol]: 192.38

Physical Properties

Property code	Value	Unit	Source
gf	89.10	kJ/mol	Joback Method
hf	-164.66	kJ/mol	Joback Method
hfus	12.87	kJ/mol	Joback Method
hvap	47.19	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	4.006		Crippen Method
mcvol	170.370	ml/mol	McGowan Method
pc	2467.81	kPa	Joback Method
rinpol	1191.00		NIST Webbook
tb	538.77	K	Joback Method
tc	764.38	K	Joback Method
tf	232.41	K	Joback Method
vc	0.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	390.78	J/mol×K	538.77	Joback Method
cpg	408.11	J/mol×K	576.37	Joback Method
cpg	424.39	J/mol×K	613.97	Joback Method
cpg	439.66	J/mol×K	651.57	Joback Method
cpg	453.96	J/mol×K	689.17	Joback Method
cpg	467.31	J/mol×K	726.78	Joback Method
cpg	479.76	J/mol×K	764.38	Joback Method

Sources

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=R155552&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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