2,6-dimethyl-4-ethyl-3,5-dithiaheptane

Inchi: InChI=1S/C9H20S2/c1-6-9(10-7(2)3)11-8(4)5/h7-9H,6H2,1-5H3
InchiKey: IEVDPNZUQCRZHC-UHFFFAOYSA-N
Formula: C9H20S2
SMILES: CCC(SC(C)C)SC(C)C
Mol. weight [g/mol]: 192.38

Physical Properties

Property code	Value	Unit	Source
gf	83.82	kJ/mol	Joback Method
hf	-161.19	kJ/mol	Joback Method
hfus	16.76	kJ/mol	Joback Method
hvap	48.10	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	4.006		Crippen Method
mcvol	170.370	ml/mol	McGowan Method
pc	2441.06	kPa	Joback Method
rinpol	1218.00		NIST Webbook
rinpol	1218.00		NIST Webbook
tb	541.56	K	Joback Method
tc	758.12	K	Joback Method
tf	214.99	K	Joback Method
vc	0.629	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	387.89	J/mol×K	541.56	Joback Method
cpg	404.50	J/mol×K	577.65	Joback Method
cpg	420.26	J/mol×K	613.75	Joback Method
cpg	435.17	J/mol×K	649.84	Joback Method
cpg	449.26	J/mol×K	685.94	Joback Method
cpg	462.52	J/mol×K	722.03	Joback Method
cpg	474.98	J/mol×K	758.12	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=R155869&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