2,4-dimethyl-3,5-dithiahexane

Inchi: InChI=1S/C6H14S2/c1-5(2)8-6(3)7-4/h5-6H,1-4H3
InchiKey: XKBOUYAAHFKBPJ-UHFFFAOYSA-N
Formula: C6H14S2
SMILES: CSC(C)SC(C)C
Mol. weight [g/mol]: 150.31

Physical Properties

Property code	Value	Unit	Source
gf	61.00	kJ/mol	Joback Method
hf	-93.99	kJ/mol	Joback Method
hfus	12.51	kJ/mol	Joback Method
hvap	41.81	kJ/mol	Joback Method
log10ws	-2.82		Crippen Method
logp	2.837		Crippen Method
mcvol	128.100	ml/mol	McGowan Method
pc	3287.81	kPa	Joback Method
rinpol	1055.00		NIST Webbook
rinpol	1055.00		NIST Webbook
tb	473.36	K	Joback Method
tc	695.84	K	Joback Method
tf	196.18	K	Joback Method
vc	0.468	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	254.40	J/mol×K	473.36	Joback Method
cpg	267.47	J/mol×K	510.44	Joback Method
cpg	279.93	J/mol×K	547.52	Joback Method
cpg	291.77	J/mol×K	584.60	Joback Method
cpg	303.01	J/mol×K	621.68	Joback Method
cpg	313.64	J/mol×K	658.76	Joback Method
cpg	323.66	J/mol×K	695.84	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R155636&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

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