2-methyl-3,6-dithiaheptane

Inchi: InChI=1S/C6H14S2/c1-6(2)8-5-4-7-3/h6H,4-5H2,1-3H3
InchiKey: FOAMPFHQZRGICO-UHFFFAOYSA-N
Formula: C6H14S2
SMILES: CSCCSC(C)C
Mol. weight [g/mol]: 150.31

Physical Properties

Property code	Value	Unit	Source
gf	63.44	kJ/mol	Joback Method
hf	-88.71	kJ/mol	Joback Method
hfus	16.03	kJ/mol	Joback Method
hvap	42.20	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	2.491		Crippen Method
mcvol	128.100	ml/mol	McGowan Method
pc	3257.86	kPa	Joback Method
rinpol	1148.00		NIST Webbook
rinpol	1148.00		NIST Webbook
tb	473.80	K	Joback Method
tc	691.06	K	Joback Method
tf	211.18	K	Joback Method
vc	0.473	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	254.21	J/mol×K	473.80	Joback Method
cpg	266.88	J/mol×K	510.01	Joback Method
cpg	278.98	J/mol×K	546.22	Joback Method
cpg	290.51	J/mol×K	582.43	Joback Method
cpg	301.47	J/mol×K	618.64	Joback Method
cpg	311.87	J/mol×K	654.85	Joback Method
cpg	321.69	J/mol×K	691.06	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=R156104&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