6,6-dimethyl-4,5-dithia-1-heptene

Inchi: InChI=1S/C7H14S2/c1-5-6-8-9-7(2,3)4/h5H,1,6H2,2-4H3
InchiKey: SHJCLWYJLALLDH-UHFFFAOYSA-N
Formula: C7H14S2
SMILES: C=CCSSC(C)(C)C
Mol. weight [g/mol]: 162.32

Physical Properties

Property code	Value	Unit	Source
gf	164.98	kJ/mol	Joback Method
hf	12.61	kJ/mol	Joback Method
hfus	13.45	kJ/mol	Joback Method
hvap	42.84	kJ/mol	Joback Method
log10ws	-3.48		Crippen Method
logp	3.352		Crippen Method
mcvol	137.890	ml/mol	McGowan Method
pc	3103.64	kPa	Joback Method
rinpol	1098.00		NIST Webbook
tb	490.57	K	Joback Method
tc	718.88	K	Joback Method
tf	238.11	K	Joback Method
vc	0.505	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.90	J/mol×K	490.57	Joback Method
cpg	295.82	J/mol×K	528.62	Joback Method
cpg	308.86	J/mol×K	566.67	Joback Method
cpg	321.07	J/mol×K	604.72	Joback Method
cpg	332.46	J/mol×K	642.78	Joback Method
cpg	343.09	J/mol×K	680.83	Joback Method
cpg	352.97	J/mol×K	718.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R157563&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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