2,4-dimethyl-3,5-dithia-7-octene

Inchi: InChI=1S/C8H16S2/c1-5-6-9-8(4)10-7(2)3/h5,7-8H,1,6H2,2-4H3
InchiKey: MZTJNVGAWXUYGR-UHFFFAOYSA-N
Formula: C8H16S2
SMILES: C=CCSC(C)SC(C)C
Mol. weight [g/mol]: 176.34

Physical Properties

Property code	Value	Unit	Source
gf	165.68	kJ/mol	Joback Method
hf	-9.84	kJ/mol	Joback Method
hfus	16.41	kJ/mol	Joback Method
hvap	45.59	kJ/mol	Joback Method
log10ws	-3.51		Crippen Method
logp	3.393		Crippen Method
mcvol	151.980	ml/mol	McGowan Method
pc	2787.66	kPa	Joback Method
rinpol	1185.00		NIST Webbook
tb	515.80	K	Joback Method
tc	735.95	K	Joback Method
tf	216.96	K	Joback Method
vc	0.560	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.79	J/mol×K	515.80	Joback Method
cpg	337.40	J/mol×K	552.49	Joback Method
cpg	351.24	J/mol×K	589.18	Joback Method
cpg	364.33	J/mol×K	625.87	Joback Method
cpg	376.68	J/mol×K	662.56	Joback Method
cpg	388.30	J/mol×K	699.26	Joback Method
cpg	399.20	J/mol×K	735.95	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=R155621&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