5-methyl-4,6-dithia-1,8-nonadiene

Inchi: InChI=1S/C8H14S2/c1-4-6-9-8(3)10-7-5-2/h4-5,8H,1-2,6-7H2,3H3
InchiKey: PJVWWOABPTYHLI-UHFFFAOYSA-N
Formula: C8H14S2
SMILES: C=CCSC(C)SCC=C
Mol. weight [g/mol]: 174.33

Physical Properties

Property code	Value	Unit	Source
gf	255.96	kJ/mol	Joback Method
hf	120.87	kJ/mol	Joback Method
hfus	18.65	kJ/mol	Joback Method
hvap	45.31	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	3.171		Crippen Method
mcvol	147.680	ml/mol	McGowan Method
pc	2890.51	kPa	Joback Method
rinpol	1224.00		NIST Webbook
tb	512.92	K	Joback Method
tc	732.91	K	Joback Method
tf	230.20	K	Joback Method
vc	0.547	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	304.23	J/mol×K	512.92	Joback Method
cpg	317.73	J/mol×K	549.58	Joback Method
cpg	330.48	J/mol×K	586.25	Joback Method
cpg	342.52	J/mol×K	622.91	Joback Method
cpg	353.85	J/mol×K	659.58	Joback Method
cpg	364.49	J/mol×K	696.24	Joback Method
cpg	374.47	J/mol×K	732.91	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=R157449&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