2,4-Dimethyl-5,6-dithia-2,7-nonadienal, 5-oxide

Other names: 2,4-dimethyl-5,6-dithia-2,7-nonadienal 5-oxide
Inchi: InChI=1S/C9H14O2S2/c1-4-5-12-13(11)9(3)6-8(2)7-10/h4-7,9H,1-3H3/b5-4+,8-6+
InchiKey: QFRRWTCSHVAIAV-DVBIZMGNSA-N
Formula: C9H14O2S2
SMILES: CC=CSS(=O)C(C)C=C(C)C=O
Mol. weight [g/mol]: 218.34

Physical Properties

Property code	Value	Unit	Source
gf	-109.76	kJ/mol	Joback Method
hf	-259.17	kJ/mol	Joback Method
hfus	28.81	kJ/mol	Joback Method
hvap	61.50	kJ/mol	Joback Method
log10ws	-2.69		Crippen Method
logp	2.451		Crippen Method
mcvol	169.210	ml/mol	McGowan Method
pc	3127.99	kPa	Joback Method
rinpol	1723.00		NIST Webbook
rinpol	1723.00		NIST Webbook
rinpol	1734.00		NIST Webbook
tb	588.80	K	Joback Method
tc	808.39	K	Joback Method
tf	264.95	K	Joback Method
vc	0.655	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	382.04	J/mol×K	588.80	Joback Method
cpg	395.31	J/mol×K	625.40	Joback Method
cpg	407.73	J/mol×K	662.00	Joback Method
cpg	419.32	J/mol×K	698.60	Joback Method
cpg	430.13	J/mol×K	735.19	Joback Method
cpg	440.19	J/mol×K	771.79	Joback Method

cpg	449.52	J/mol×K	808.39	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=U322313&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

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