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

Inchi: InChI=1S/C9H14OS2/c1-4-5-11-12-9(3)6-8(2)7-10/h4-7,9H,1-3H3/b5-4+,8-6+
InchiKey: HEONUJXIZOQNOR-DVBIZMGNSA-N
Formula: C9H14OS2
SMILES: CC=CSSC(C)C=C(C)C=O
Mol. weight [g/mol]: 202.34

Physical Properties

Property code	Value	Unit	Source
gf	141.07	kJ/mol	Joback Method
hf	-11.56	kJ/mol	Joback Method
hfus	25.19	kJ/mol	Joback Method
hvap	55.59	kJ/mol	Joback Method
log10ws	-3.94		Crippen Method
logp	3.435		Crippen Method
mcvol	163.340	ml/mol	McGowan Method
pc	2899.85	kPa	Joback Method
rinpol	1529.00		NIST Webbook
rinpol	1563.00		NIST Webbook
rinpol	1536.00		NIST Webbook
rinpol	1529.00		NIST Webbook
tb	599.30	K	Joback Method
tc	832.77	K	Joback Method
tf	262.87	K	Joback Method
vc	0.620	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	366.64	J/mol×K	599.30	Joback Method
cpg	379.88	J/mol×K	638.21	Joback Method
cpg	392.23	J/mol×K	677.12	Joback Method
cpg	403.74	J/mol×K	716.03	Joback Method
cpg	414.45	J/mol×K	754.94	Joback Method
cpg	424.42	J/mol×K	793.86	Joback Method

cpg	433.69	J/mol×K	832.77	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=U322305&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