4,6-dithia-1,8-nonadiene

Inchi: InChI=1S/C7H12S2/c1-3-5-8-7-9-6-4-2/h3-4H,1-2,5-7H2
InchiKey: QTUCHGYIDKFWSU-UHFFFAOYSA-N
Formula: C7H12S2
SMILES: C=CCSCSCC=C
Mol. weight [g/mol]: 160.30
CAS: 18068-26-3

Physical Properties

Property code	Value	Unit	Source
gf	249.98	kJ/mol	Joback Method
hf	146.79	kJ/mol	Joback Method
hfus	19.59	kJ/mol	Joback Method
hvap	43.47	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.782		Crippen Method
mcvol	133.590	ml/mol	McGowan Method
pc	3184.73	kPa	Joback Method
rinpol	1193.00		NIST Webbook
rinpol	1193.00		NIST Webbook
tb	490.48	K	Joback Method
tc	709.02	K	Joback Method
tf	233.93	K	Joback Method
vc	0.497	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	261.19	J/mol×K	490.48	Joback Method
cpg	273.20	J/mol×K	526.90	Joback Method
cpg	284.57	J/mol×K	563.33	Joback Method
cpg	295.32	J/mol×K	599.75	Joback Method
cpg	305.46	J/mol×K	636.17	Joback Method
cpg	315.01	J/mol×K	672.60	Joback Method
cpg	323.97	J/mol×K	709.02	Joback Method

Sources

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=C18068263&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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