4,5-dithia-1-heptene

Inchi: InChI=1S/C5H10S2/c1-3-5-7-6-4-2/h3H,1,4-5H2,2H3
InchiKey: DJLRNCWMAKPXJF-UHFFFAOYSA-N
Formula: C5H10S2
SMILES: C=CCSSCC
Mol. weight [g/mol]: 134.26

Physical Properties

Property code	Value	Unit	Source
gf	145.30	kJ/mol	Joback Method
hf	62.64	kJ/mol	Joback Method
hfus	15.69	kJ/mol	Joback Method
hvap	39.69	kJ/mol	Joback Method
log10ws	-2.53		Crippen Method
logp	2.574		Crippen Method
mcvol	109.710	ml/mol	McGowan Method
pc	3801.00	kPa	Joback Method
rinpol	1008.00		NIST Webbook
rinpol	1008.00		NIST Webbook
tb	448.04	K	Joback Method
tc	668.29	K	Joback Method
tf	213.15	K	Joback Method
vc	0.405	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	197.76	J/mol×K	448.04	Joback Method
cpg	207.91	J/mol×K	484.75	Joback Method
cpg	217.59	J/mol×K	521.46	Joback Method
cpg	226.80	J/mol×K	558.17	Joback Method
cpg	235.54	J/mol×K	594.88	Joback Method
cpg	243.82	J/mol×K	631.59	Joback Method
cpg	251.64	J/mol×K	668.29	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=R156986&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