2,5-dithiaheptane

Inchi: InChI=1S/C5H12S2/c1-3-7-5-4-6-2/h3-5H2,1-2H3
InchiKey: BKPCLDKCWGHGLQ-UHFFFAOYSA-N
Formula: C5H12S2
SMILES: CCSCCSC
Mol. weight [g/mol]: 136.28

Physical Properties

Property code	Value	Unit	Source
gf	57.46	kJ/mol	Joback Method
hf	-62.79	kJ/mol	Joback Method
hfus	16.97	kJ/mol	Joback Method
hvap	40.36	kJ/mol	Joback Method
log10ws	-1.68		Crippen Method
logp	2.103		Crippen Method
mcvol	114.010	ml/mol	McGowan Method
pc	3611.55	kPa	Joback Method
rinpol	1105.00		NIST Webbook
tb	451.36	K	Joback Method
tc	666.63	K	Joback Method
tf	214.91	K	Joback Method
vc	0.423	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	213.79	J/mol×K	451.36	Joback Method
cpg	224.75	J/mol×K	487.24	Joback Method
cpg	235.26	J/mol×K	523.12	Joback Method
cpg	245.30	J/mol×K	558.99	Joback Method
cpg	254.88	J/mol×K	594.87	Joback Method
cpg	264.00	J/mol×K	630.75	Joback Method
cpg	272.66	J/mol×K	666.63	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=R155770&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