2,2,6-trimethyl-3,4-dithiaheptane

Inchi: InChI=1S/C8H18S2/c1-7(2)6-9-10-8(3,4)5/h7H,6H2,1-5H3
InchiKey: ZVSGZORIEHXCDY-UHFFFAOYSA-N
Formula: C8H18S2
SMILES: CC(C)CSSC(C)(C)C
Mol. weight [g/mol]: 178.36

Physical Properties

Property code	Value	Unit	Source
gf	83.12	kJ/mol	Joback Method
hf	-138.74	kJ/mol	Joback Method
hfus	13.80	kJ/mol	Joback Method
hvap	45.35	kJ/mol	Joback Method
log10ws	-3.80		Crippen Method
logp	3.822		Crippen Method
mcvol	156.280	ml/mol	McGowan Method
pc	2698.60	kPa	Joback Method
rinpol	1159.00		NIST Webbook
rinpol	1159.00		NIST Webbook
tb	516.33	K	Joback Method
tc	740.84	K	Joback Method
tf	236.14	K	Joback Method
vc	0.575	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	344.19	J/mol×K	516.33	Joback Method
cpg	360.24	J/mol×K	553.75	Joback Method
cpg	375.34	J/mol×K	591.17	Joback Method
cpg	389.53	J/mol×K	628.59	Joback Method
cpg	402.82	J/mol×K	666.00	Joback Method
cpg	415.26	J/mol×K	703.42	Joback Method
cpg	426.87	J/mol×K	740.84	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R155285&Units=SI
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

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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