2-methyl-3,5-dithianonane

Inchi: InChI=1S/C8H18S2/c1-4-5-6-9-7-10-8(2)3/h8H,4-7H2,1-3H3
InchiKey: MDQULDJIVAIFSF-UHFFFAOYSA-N
Formula: C8H18S2
SMILES: CCCCSCSC(C)C
Mol. weight [g/mol]: 178.36

Physical Properties

Property code	Value	Unit	Source
gf	80.28	kJ/mol	Joback Method
hf	-129.99	kJ/mol	Joback Method
hfus	21.21	kJ/mol	Joback Method
hvap	46.65	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	3.619		Crippen Method
mcvol	156.280	ml/mol	McGowan Method
pc	2646.11	kPa	Joback Method
rinpol	1276.00		NIST Webbook
tb	519.56	K	Joback Method
tc	730.16	K	Joback Method
tf	233.72	K	Joback Method
vc	0.586	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	341.00	J/mol×K	519.56	Joback Method
cpg	355.88	J/mol×K	554.66	Joback Method
cpg	370.06	J/mol×K	589.76	Joback Method
cpg	383.53	J/mol×K	624.86	Joback Method
cpg	396.31	J/mol×K	659.96	Joback Method
cpg	408.41	J/mol×K	695.06	Joback Method
cpg	419.83	J/mol×K	730.16	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=R156080&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