2-methyl-5-thianonane

Inchi: InChI=1S/C9H20S/c1-4-5-7-10-8-6-9(2)3/h9H,4-8H2,1-3H3
InchiKey: PSEUPOGUWGHLIJ-UHFFFAOYSA-N
Formula: C9H20S
SMILES: CCCCSCCC(C)C
Mol. weight [g/mol]: 160.32

Physical Properties

Property code	Value	Unit	Source
gf	55.58	kJ/mol	Joback Method
hf	-192.50	kJ/mol	Joback Method
hfus	19.67	kJ/mol	Joback Method
hvap	42.06	kJ/mol	Joback Method
log10ws	-3.23		Crippen Method
logp	3.566		Crippen Method
mcvol	154.020	ml/mol	McGowan Method
pc	2363.37	kPa	Joback Method
rinpol	1140.00		NIST Webbook
rinpol	1140.00		NIST Webbook
rinpol	1140.00		NIST Webbook
rinpol	1140.00		NIST Webbook
tb	473.66	K	Joback Method
tc	661.48	K	Joback Method
tf	210.59	K	Joback Method
vc	0.588	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	330.57	J/mol×K	473.66	Joback Method
cpg	345.86	J/mol×K	504.96	Joback Method
cpg	360.50	J/mol×K	536.27	Joback Method
cpg	374.52	J/mol×K	567.57	Joback Method
cpg	387.92	J/mol×K	598.87	Joback Method
cpg	400.72	J/mol×K	630.17	Joback Method

cpg	412.93	J/mol×K	661.48	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R156293&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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