2,3-dimethyl-4-thianonane

Inchi: InChI=1S/C10H22S/c1-5-6-7-8-11-10(4)9(2)3/h9-10H,5-8H2,1-4H3
InchiKey: SLWLCOPCNCAVOJ-UHFFFAOYSA-N
Formula: C10H22S
SMILES: CCCCCSC(C)C(C)C
Mol. weight [g/mol]: 174.35

Physical Properties

Property code	Value	Unit	Source
gf	61.56	kJ/mol	Joback Method
hf	-218.42	kJ/mol	Joback Method
hfus	18.74	kJ/mol	Joback Method
hvap	43.89	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	3.954		Crippen Method
mcvol	168.110	ml/mol	McGowan Method
pc	2173.43	kPa	Joback Method
rinpol	1204.00		NIST Webbook
rinpol	1204.00		NIST Webbook
rinpol	1204.00		NIST Webbook
rinpol	1204.00		NIST Webbook
tb	496.10	K	Joback Method
tc	685.89	K	Joback Method
tf	206.86	K	Joback Method
vc	0.637	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	376.28	J/mol×K	496.10	Joback Method
cpg	392.87	J/mol×K	527.73	Joback Method
cpg	408.74	J/mol×K	559.36	Joback Method
cpg	423.89	J/mol×K	591.00	Joback Method
cpg	438.36	J/mol×K	622.63	Joback Method
cpg	452.14	J/mol×K	654.26	Joback Method

cpg	465.27	J/mol×K	685.89	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R155527&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