2,2,8-trimethyl-3,4-dithianonane

Inchi: InChI=1S/C10H22S2/c1-9(2)7-6-8-11-12-10(3,4)5/h9H,6-8H2,1-5H3
InchiKey: YFIABJPNNHDMKM-UHFFFAOYSA-N
Formula: C10H22S2
SMILES: CC(C)CCCSSC(C)(C)C
Mol. weight [g/mol]: 206.41

Physical Properties

Property code	Value	Unit	Source
gf	99.96	kJ/mol	Joback Method
hf	-180.02	kJ/mol	Joback Method
hfus	18.98	kJ/mol	Joback Method
hvap	49.80	kJ/mol	Joback Method
log10ws	-4.64		Crippen Method
logp	4.603		Crippen Method
mcvol	184.460	ml/mol	McGowan Method
pc	2231.30	kPa	Joback Method
rinpol	1257.00		NIST Webbook
tb	562.09	K	Joback Method
tc	778.85	K	Joback Method
tf	258.68	K	Joback Method
vc	0.686	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	438.52	J/mol×K	562.09	Joback Method
cpg	456.09	J/mol×K	598.22	Joback Method
cpg	472.63	J/mol×K	634.34	Joback Method
cpg	488.18	J/mol×K	670.47	Joback Method
cpg	502.78	J/mol×K	706.59	Joback Method
cpg	516.47	J/mol×K	742.72	Joback Method
cpg	529.26	J/mol×K	778.85	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R155309&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