3,7-dimethyl-4,6-dithianonane

Inchi: InChI=1S/C9H20S2/c1-5-8(3)10-7-11-9(4)6-2/h8-9H,5-7H2,1-4H3
InchiKey: UXWQSLDEJIEENH-UHFFFAOYSA-N
Formula: C9H20S2
SMILES: CCC(C)SCSC(C)CC
Mol. weight [g/mol]: 192.38

Physical Properties

Property code	Value	Unit	Source
gf	86.26	kJ/mol	Joback Method
hf	-155.91	kJ/mol	Joback Method
hfus	20.28	kJ/mol	Joback Method
hvap	48.49	kJ/mol	Joback Method
log10ws	-4.08		Crippen Method
logp	4.007		Crippen Method
mcvol	170.370	ml/mol	McGowan Method
pc	2421.88	kPa	Joback Method
rinpol	1320.00		NIST Webbook
tb	542.00	K	Joback Method
tc	753.86	K	Joback Method
tf	229.99	K	Joback Method
vc	0.635	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	387.59	J/mol×K	542.00	Joback Method
cpg	403.78	J/mol×K	577.31	Joback Method
cpg	419.15	J/mol×K	612.62	Joback Method
cpg	433.73	J/mol×K	647.93	Joback Method
cpg	447.52	J/mol×K	683.24	Joback Method
cpg	460.55	J/mol×K	718.55	Joback Method
cpg	472.80	J/mol×K	753.86	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R156575&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