2,3,6,7-tetramethyl-4,5-dithiaoctane

Inchi: InChI=1S/C10H22S2/c1-7(2)9(5)11-12-10(6)8(3)4/h7-10H,1-6H3
InchiKey: NXURYLWXQQBBPT-UHFFFAOYSA-N
Formula: C10H22S2
SMILES: CC(C)C(C)SSC(C)C(C)C
Mol. weight [g/mol]: 206.41

Physical Properties

Property code	Value	Unit	Source
gf	89.80	kJ/mol	Joback Method
hf	-187.11	kJ/mol	Joback Method
hfus	15.82	kJ/mol	Joback Method
hvap	49.94	kJ/mol	Joback Method
log10ws	-4.51		Crippen Method
logp	4.457		Crippen Method
mcvol	184.460	ml/mol	McGowan Method
pc	2241.88	kPa	Joback Method
rinpol	1348.00		NIST Webbook
tb	564.00	K	Joback Method
tc	781.56	K	Joback Method
tf	211.26	K	Joback Method
vc	0.679	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	436.37	J/mol×K	564.00	Joback Method
cpg	454.17	J/mol×K	600.26	Joback Method
cpg	471.01	J/mol×K	636.52	Joback Method
cpg	486.92	J/mol×K	672.78	Joback Method
cpg	501.91	J/mol×K	709.04	Joback Method
cpg	515.99	J/mol×K	745.30	Joback Method
cpg	529.18	J/mol×K	781.56	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R155478&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