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

Inchi: InChI=1S/C10H22S2/c1-9(2,3)7-11-12-8-10(4,5)6/h7-8H2,1-6H3
InchiKey: SEZZRXXPRCBINH-UHFFFAOYSA-N
Formula: C10H22S2
SMILES: CC(C)(C)CSSCC(C)(C)C
Mol. weight [g/mol]: 206.41
CAS: 37552-63-9

Physical Properties

Property code	Value	Unit	Source
gf	105.24	kJ/mol	Joback Method
hf	-183.49	kJ/mol	Joback Method
hfus	15.09	kJ/mol	Joback Method
hvap	48.90	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	4.460		Crippen Method
mcvol	184.460	ml/mol	McGowan Method
pc	2254.67	kPa	Joback Method
rinpol	1348.00		NIST Webbook
tb	559.30	K	Joback Method
tc	784.94	K	Joback Method
tf	276.10	K	Joback Method
vc	0.681	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	441.33	J/mol×K	559.30	Joback Method
cpg	459.58	J/mol×K	596.91	Joback Method
cpg	476.62	J/mol×K	634.51	Joback Method
cpg	492.50	J/mol×K	672.12	Joback Method
cpg	507.28	J/mol×K	709.72	Joback Method
cpg	521.03	J/mol×K	747.33	Joback Method
cpg	533.81	J/mol×K	784.94	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C37552639&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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