

Tetramethyltetrathiafulvalene

Other names:	1,3-Dithiole,2-(4,5-dimethyl-1,3-dithiol-2-ylidene)-4,5-dimethyl-4,5,4',5'-Tetramethyl-[2,2']bi[[1,3]dithiolindene]
Inchi:	InChI=1S/C10H12S4/c1-5-6(2)12-9(11-5)10-13-7(3)8(4)14-10/h1-4H3
InchiKey:	HGOTVGUTJPNVDR-UHFFFAOYSA-N
Formula:	C10H12S4
SMILES:	CC1=C(C)SC(=C2SC(C)=C(C)S2)S1
Mol. weight [g/mol]:	260.46
CAS:	50708-37-7

Physical Properties

Property code	Value	Unit	Source
gf	313.38	kJ/mol	Joback Method
hf	197.47	kJ/mol	Joback Method
hfus	23.34	kJ/mol	Joback Method
hvap	67.08	kJ/mol	Joback Method
ie	6.03	eV	NIST Webbook
ie	6.40	eV	NIST Webbook
log10ws	-6.86		Crippen Method
logp	5.576		Crippen Method
mcvol	182.540	ml/mol	McGowan Method
pc	3235.66	kPa	Joback Method
tb	686.78	K	Joback Method
tc	972.62	K	Joback Method
tf	643.94	K	Joback Method
vc	0.622	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.31	J/molxK	686.78	Joback Method
cpg	422.56	J/molxK	734.42	Joback Method
cpg	434.87	J/molxK	782.06	Joback Method
cpg	446.32	J/molxK	829.70	Joback Method
cpg	457.02	J/molxK	877.34	Joback Method

cpg	467.04	J/mol×K	924.98	Joback Method
cpg	476.49	J/mol×K	972.62	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=C50708377&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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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