

[1,2]Dithiolo[1,5-b][1,2]dithiole-7-SIV

Other names:	1,6,6a-Trithia(6a-SIV)pentalene
	1,6,6a-Trithiapentalene-6aS
	1,6,6a-Trithiapentalene-6«alpha»-S(IV)
	1,6,6aS(IV)-Trithiapentalene
	6a-Thiathiophthene
	Meribicyclo-1,3-epidithiopenta-1,3-diene-5-thial
	Thiathiophthen
	Thiathiophthene
	Thiothiophthene
	Trithiapentalene
Inchi:	[1,2]Dithiolo[1,5-b][1,2]dithiole
InchiKey:	InChI=1S/C5H4S3/c1-3-6-8-5(1)2-4-7-8/h1-4H
Formula:	JUEJPBZMWHMMPS-UHFFFAOYSA-N
SMILES:	C5H4S3
Mol. weight [g/mol]:	C1=CC2=S(S1)SC=C2
	160.29

Physical Properties

Property code	Value	Unit	Source
hfus	10.59	kJ/mol	Joback Method
ie	8.11	eV	NIST Webbook
logp	2.779		Crippen Method
mcvol	100.040	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	175.49	J/mol×K	492.23	Joback Method
cpg	185.10	J/mol×K	539.97	Joback Method
cpg	193.71	J/mol×K	587.70	Joback Method
cpg	201.43	J/mol×K	635.44	Joback Method
cpg	208.34	J/mol×K	683.17	Joback Method
cpg	214.54	J/mol×K	730.91	Joback Method
cpg	220.13	J/mol×K	778.64	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C252095&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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