

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

Other names:	1,6,6a-SIV-trithiapentalene, 2,5-diphenyl- 2,5-Diphenyl-1,6,6a-SIV-trithiapentalene 2,5-Diphenyl-6a-thiathiophthene 2,5-Diphenyl-1,6,6a-«delta»-4-trithiapentalene 1,6,6A(IVS)-Trithiapentalene, 2,5-diphenyl-
Inchi:	InChI=1S/C17H12S3/c1-3-7-13(8-4-1)16-11-15-12-17(19-20(15)18-16)14-9-5-2-6-10-14/
InchiKey:	SRITYXMHFJHYIZ-UHFFFAOYSA-N
Formula:	C17H12S3
SMILES:	C1=C(c2ccccc2)SS2=C1C=C(c1ccccc1)S2
Mol. weight [g/mol]:	312.47
CAS:	1033-90-5

Physical Properties

Property code	Value	Unit	Source
gf	543.01	kJ/mol	Joback Method
hf	442.82	kJ/mol	Joback Method
hfus	28.97	kJ/mol	Joback Method
hvap	79.08	kJ/mol	Joback Method
ie	7.39	eV	NIST Webbook
log10ws	-7.19		Crippen Method
logp	5.833		Crippen Method
mcvol	221.600	ml/mol	McGowan Method
pc	2989.32	kPa	Joback Method
tb	830.11	K	Joback Method
tc	1148.75	K	Joback Method
tf	644.95	K	Joback Method
vc	0.783	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	573.95	J/mol×K	830.11	Joback Method
cpg	588.88	J/mol×K	883.22	Joback Method
cpg	602.31	J/mol×K	936.32	Joback Method

cpg	614.49	J/mol×K	989.43	Joback Method
cpg	625.69	J/mol×K	1042.54	Joback Method
cpg	636.17	J/mol×K	1095.65	Joback Method
cpg	646.20	J/mol×K	1148.75	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1033905&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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