

5-hydroxy-1,2-dithiacyclooctane

Other names:	1,2-Dithiacyclooctane, 5-hydroxy
Inchi:	InChI=1S/C6H12OS2/c7-6-2-1-4-8-9-5-3-6/h6-7H,1-5H2
InchiKey:	FGYSGNWYOAYLOE-UHFFFAOYSA-N
Formula:	C6H12OS2
SMILES:	OC1CCCSSCC1
Mol. weight [g/mol]:	164.29

Physical Properties

Property code	Value	Unit	Source
gf	-57.21	kJ/mol	Joback Method
hf	-186.88	kJ/mol	Joback Method
hfus	10.33	kJ/mol	Joback Method
hvap	58.03	kJ/mol	Joback Method
log10ws	-2.36		Crippen Method
logp	1.913		Crippen Method
mvol	123.110	ml/mol	McGowan Method
pc	4697.74	kPa	Joback Method
rinpol	1221.00		NIST Webbook
tb	552.61	K	Joback Method
tc	789.93	K	Joback Method
tf	385.44	K	Joback Method
vc	0.400	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.99	J/molxK	552.61	Joback Method
cpg	290.46	J/molxK	592.16	Joback Method
cpg	304.01	J/molxK	631.72	Joback Method
cpg	316.66	J/molxK	671.27	Joback Method
cpg	328.43	J/molxK	710.82	Joback Method
cpg	339.33	J/molxK	750.38	Joback Method
cpg	349.36	J/molxK	789.93	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R82334&Units=SI

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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