

Dihydro-2(3H)-thiophenthione

Inchi:	InChI=1S/C4H6S2/c5-4-2-1-3-6-4/h1-3H2
InchiKey:	SMRSQGJONQYPSA-UHFFFAOYSA-N
Formula:	C4H6S2
SMILES:	S=C1CCCS1
Mol. weight [g/mol]:	118.22

Physical Properties

Property code	Value	Unit	Source
gf	157.77	kJ/mol	Joback Method
hf	115.29	kJ/mol	Joback Method
hfus	8.67	kJ/mol	Joback Method
hvap	38.35	kJ/mol	Joback Method
log10ws	-2.13		Crippen Method
logp	1.841		Crippen Method
mcvol	84.760	ml/mol	McGowan Method
pc	5644.74	kPa	Joback Method
ripol	1720.00		NIST Webbook
ripol	1720.00		NIST Webbook
tb	431.34	K	Joback Method
tc	677.47	K	Joback Method
tf	297.10	K	Joback Method
vc	0.285	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	139.07	J/molxK	431.34	Joback Method
cpg	148.48	J/molxK	472.36	Joback Method
cpg	157.05	J/molxK	513.38	Joback Method
cpg	164.87	J/molxK	554.41	Joback Method
cpg	172.00	J/molxK	595.43	Joback Method
cpg	178.51	J/molxK	636.45	Joback Method
cpg	184.47	J/molxK	677.47	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=R301661&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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