1-(4-Methyl-4H-[1,3]dithiin-2-yl)-propane-2-thiol

Inchi: InChI=1S/C8H14S3/c1-6(9)5-8-10-4-3-7(2)11-8/h3-4,6-9H,5H2,1-2H3
InchiKey: KIZYPBJKLBKTGJ-UHFFFAOYSA-N
Formula: C8H14S3
SMILES: CC(S)CC1SC=CC(C)S1
Mol. weight [g/mol]: 206.39

Physical Properties

Property code	Value	Unit	Source
gf	169.85	kJ/mol	Joback Method
hf	7.03	kJ/mol	Joback Method
hfus	18.44	kJ/mol	Joback Method
hvap	51.79	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	3.403		Crippen Method
mcvol	157.470	ml/mol	McGowan Method
pc	3388.08	kPa	Joback Method
rinpol	1530.00		NIST Webbook
tb	554.56	K	Joback Method
tc	816.80	K	Joback Method
tf	372.18	K	Joback Method
vc	0.541	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.42	J/mol×K	554.56	Joback Method
cpg	363.71	J/mol×K	598.27	Joback Method
cpg	379.78	J/mol×K	641.97	Joback Method
cpg	394.67	J/mol×K	685.68	Joback Method
cpg	408.42	J/mol×K	729.39	Joback Method
cpg	421.08	J/mol×K	773.09	Joback Method
cpg	432.69	J/mol×K	816.80	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R487275&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume