Hydrazinecarbodithioic acid, 2-phenyl-, methyl ester

Other names: 3-Phenyldithiocarbazic acid methyl ester
Inchi: InChI=1S/C8H10N2S2/c1-12-8(11)10-9-7-5-3-2-4-6-7/h2-6,9H,1H3,(H,10,11)
InchiKey: SZCVCDOFDCMDRN-UHFFFAOYSA-N
Formula: C8H10N2S2
SMILES: CSC(=S)NNc1ccccc1
Mol. weight [g/mol]: 198.31
CAS: 50878-38-1

Physical Properties

Property code	Value	Unit	Source
gf	457.85	kJ/mol	Joback Method
hf	323.39	kJ/mol	Joback Method
hfus	29.45	kJ/mol	Joback Method
hvap	62.10	kJ/mol	Joback Method
ie	8.47	eV	NIST Webbook
log10ws	-3.31		Crippen Method
logp	2.251		Crippen Method
mcvol	148.180	ml/mol	McGowan Method
pc	4328.25	kPa	Joback Method
tb	648.28	K	Joback Method
tc	906.30	K	Joback Method
tf	380.33	K	Joback Method
vc	0.535	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	338.34	J/mol×K	648.28	Joback Method
cpg	349.89	J/mol×K	691.28	Joback Method
cpg	360.42	J/mol×K	734.29	Joback Method
cpg	370.02	J/mol×K	777.29	Joback Method
cpg	378.80	J/mol×K	820.30	Joback Method
cpg	386.86	J/mol×K	863.30	Joback Method
cpg	394.29	J/mol×K	906.30	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=C50878381&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