Benzenecarboximidothioic acid, N-methyl-, methyl ester

Inchi: InChI=1S/C9H11NS/c1-10-9(11-2)8-6-4-3-5-7-8/h3-7H,1-2H3/b10-9-
InchiKey: PCHKPGSXUAGLCS-KTKRTIGZSA-N
Formula: C9H11NS
SMILES: CN=C(SC)c1ccccc1
Mol. weight [g/mol]: 165.25
CAS: 40780-82-3

Physical Properties

Property code	Value	Unit	Source
hf	121.74	kJ/mol	Joback Method
hvap	48.11	kJ/mol	Joback Method
log10ws	-2.34		Crippen Method
logp	2.426		Crippen Method
mcvol	135.940	ml/mol	McGowan Method
pc	2973.04	kPa	Joback Method
tb	577.34	K	Joback Method
tc	831.45	K	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=C40780823&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hf: Enthalpy of formation 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature