Butyrimidicthio acid, n-phenyl-, ehtyl ester

Inchi: InChI=1S/C12H17NS/c1-3-8-12(14-4-2)13-11-9-6-5-7-10-11/h5-7,9-10H,3-4,8H2,1-2H3/b
InchiKey: UWUDNZHWOOEBGE-SEYXRHQNSA-N
Formula: C12H17NS
SMILES: CCCC(=Nc1ccccc1)SCC
Mol. weight [g/mol]: 207.34
CAS: 19255-90-4

Physical Properties

Property code	Value	Unit	Source
hf	59.82	kJ/mol	Joback Method
hvap	54.79	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	4.270		Crippen Method
mcvol	178.210	ml/mol	McGowan Method
pc	2220.80	kPa	Joback Method
tb	645.98	K	Joback Method
tc	883.89	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C19255904&Units=SI
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

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