2-Ethyl-6-(1-methylpropyl)phenyl isothiocyanate

Inchi: InChI=1S/C13H17NS/c1-4-10(3)12-8-6-7-11(5-2)13(12)14-9-15/h6-8,10H,4-5H2,1-3H3
InchiKey: VXVNYWWOXYECKU-UHFFFAOYSA-N
Formula: C13H17NS
SMILES: CCc1cccc(C(C)CC)c1N=C=S
Mol. weight [g/mol]: 219.35
CAS: 66609-02-7

Physical Properties

Property code	Value	Unit	Source
hf	180.73	kJ/mol	Joback Method
hvap	58.18	kJ/mol	Joback Method
log10ws	-4.80		Crippen Method
logp	4.497		Crippen Method
mcvol	188.000	ml/mol	McGowan Method
pc	2193.84	kPa	Joback Method
tb	678.99	K	Joback Method
tc	918.49	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=C66609027&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