Benzene, 1-(1-isocyanato-1-methylethyl)-3-(1-methylethenyl

Other names: 3-Isopropenyl-«alpha»,«alpha»-dimethylbenzyl isocyanate
alpha,alpha-Dimethyl meta-isopropenyl benzyl isocyanate
1-(1-isocyanato-1-methylethyl)-3-(1-methylethenyl)benzene

Inchi: InChI=1S/C13H15NO/c1-10(2)11-6-5-7-12(8-11)13(3,4)14-9-15/h5-8H,1H2,2-4H3

InchiKey: ZVEMLYIXBCTVOF-UHFFFAOYSA-N

Formula: C13H15NO

SMILES: C=C(C)c1cccc(C(C)(C)N=C=O)c1

Mol. weight [g/mol]: 201.26

CAS: 2094-99-7

Physical Properties

Property code	Value	Unit	Source
hf	14.89	kJ/mol	Joback Method
hvap	55.12	kJ/mol	Joback Method
log10ws	-8.02		Crippen Method
logp	3.291		Crippen Method
mcvol	173.220	ml/mol	McGowan Method
pc	2475.19	kPa	Joback Method
tb	588.50	K	Joback Method
tc	814.26	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2094997&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