2-Tert-butyl-6-methylphenyl isocyanate

Inchi: InChI=1S/C12H15NO/c1-9-6-5-7-10(12(2,3)4)11(9)13-8-14/h5-7H,1-4H3
InchiKey: VCHAHDOWZAYVEM-UHFFFAOYSA-N
Formula: C12H15NO
SMILES: Cc1cccc(C(C)(C)C)c1N=C=O
Mol. weight [g/mol]: 189.25
CAS: 13680-30-3

Physical Properties

Property code	Value	Unit	Source
hf	-91.58	kJ/mol	Joback Method
hvap	54.14	kJ/mol	Joback Method
log10ws	-7.74		Crippen Method
logp	3.260		Crippen Method
mcvol	163.430	ml/mol	McGowan Method
pc	2561.10	kPa	Joback Method
tb	574.04	K	Joback Method
tc	796.15	K	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.29900e+01
Coeff. B	-3.79496e+03
Coeff. C	-8.43620e+01
Temperature range (K), min.	383.12
Temperature range (K), max.	578.59

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13680303&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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

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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature