2,6-Dimethylphenyl isocyanate

Other names: Benzene, 2-isocyanato-1,3-dimethyl-
Inchi: InChI=1S/C9H9NO/c1-7-4-3-5-8(2)9(7)10-6-11/h3-5H,1-2H3
InchiKey: YQLRKXVEALTVCZ-UHFFFAOYSA-N
Formula: C9H9NO
SMILES: Cc1cccc(C)c1N=C=O
Mol. weight [g/mol]: 147.17
CAS: 28556-81-2

Physical Properties

Property code	Value	Unit	Source
hf	-20.91	kJ/mol	Joback Method
hvap	48.76	kJ/mol	Joback Method
log10ws	-6.91		Crippen Method
logp	2.271		Crippen Method
mcvol	121.160	ml/mol	McGowan Method
pc	3431.89	kPa	Joback Method
tb	508.63	K	Joback Method
tc	728.49	K	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	8.79270e+00
Coeff. B	-1.83729e+03
Coeff. C	-4.02990e+01
Temperature range (K), min.	256.32
Temperature range (K), max.	568.07

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C28556812&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
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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature