2,3-Dimethylphenylisocyanate

Other names: 2,3-dimethylphenyl isocyanate
Inchi: InChI=1S/C9H9NO/c1-7-4-3-5-9(8(7)2)10-6-11/h3-5H,1-2H3
InchiKey: KNHJIEOCVVIBIV-UHFFFAOYSA-N
Formula: C9H9NO
SMILES: Cc1cccc(N=C=O)c1C
Mol. weight [g/mol]: 147.18
CAS: 1591-99-7

Physical Properties

Property code	Value	Unit	Source
af	0.4639		Cheméo Relay (1.0)
gf	124.29	kJ/mol	Cheméo Relay (1.0, beta)
hf	-34.38	kJ/mol	Cheméo Relay (1.0)
hvap	53.32	kJ/mol	Cheméo Relay (1.0)
ie	8.44	eV	Cheméo Relay (1.0)
log10ws	-2.65		Cheméo Relay (1.0)
logp	2.271		Crippen Method
mcvol	121.160	ml/mol	McGowan Method
pc	3431.89	kPa	Joback Method
tb	469.34	K	Cheméo Relay (1.0)
tc	709.22	K	Cheméo Relay (1.0)
tf	301.22	K	Cheméo Relay (1.0)
vc	0.428	m3/kmol	Cheméo Relay (1.0)

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.51367e+01
Coeff. B	-4.24003e+03
Coeff. C	-7.73230e+01
Temperature range (K), min.	362.87
Temperature range (K), max.	508.87

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1591997&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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
tf:	Normal melting (fusion) point
vc:	Critical Volume