

2-Carboethoxyphenyl isocyanate

Other names:	2-Ethoxycarbonylphenyl isocyanate 2-Carboethoxyphenyl isocyanate
Inchi:	InChI=1S/C10H9NO3/c1-2-14-10(13)8-5-3-4-6-9(8)11-7-12/h3-6H,2H2,1H3
InchiKey:	HXVGHXDQGUPUKY-UHFFFAOYSA-N
Formula:	C10H9NO3
SMILES:	CCOC(=O)c1ccccc1N=C=O
Mol. weight [g/mol]:	191.18
CAS:	76393-16-3

Physical Properties

Property code	Value	Unit	Source
hf	-274.88	kJ/mol	Joback Method
hvap	59.48	kJ/mol	Joback Method
log10ws	-6.62		Crippen Method
logp	1.831		Crippen Method
mcvol	142.690	ml/mol	McGowan Method
pc	3295.37	kPa	Joback Method
tb	602.82	K	Joback Method
tc	823.32	K	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C76393163&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature

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