2-Ethoxycarbonylphenylisocyanate

Other names: 2-Ethoxycarbonylphenyl isocyanate
2-Carbethoxyphenyl 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]: 191.19

Physical Properties

Property code	Value	Unit	Source
af	0.5878		Cheméo Relay (1.0)
hf	-328.29	kJ/mol	Cheméo Relay (1.0)
hvap	64.37	kJ/mol	Cheméo Relay (1.0)
ie	8.77	eV	Cheméo Relay (1.0)
log10ws	-2.97		Cheméo Relay (1.0)
logp	1.831		Crippen Method
mcvol	142.690	ml/mol	McGowan Method
pc	3295.37	kPa	Joback Method
tb	531.22	K	Cheméo Relay (1.0)
tc	738.12	K	Cheméo Relay (1.0)
tf	277.38	K	Cheméo Relay (1.0)

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):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C76393163&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point