Ethyl-m-phenylenediisocyanate

Inchi: InChI=1S/C10H8N2O2/c1-2-8-3-4-9(11-6-13)5-10(8)12-7-14/h3-5H,2H2,1H3
InchiKey: FHGPADAQQRYSEH-UHFFFAOYSA-N
Formula: C10H8N2O2
SMILES: CCc1ccc(N=C=O)cc1N=C=O
Mol. weight [g/mol]: 188.18
CAS: 64711-83-7

Physical Properties

Property code	Value	Unit	Source
chl	-4883.00 ± 3.00	kJ/mol	NIST Webbook
hf	-135.00 ± 3.00	kJ/mol	NIST Webbook
hfl	-196.00 ± 3.00	kJ/mol	NIST Webbook
hvap	61.10 ± 0.80	kJ/mol	NIST Webbook
log10ws	-11.24		Crippen Method
logp	2.184		Crippen Method
mcvol	142.500	ml/mol	McGowan Method
pc	3345.11	kPa	Joback Method
tb	598.18	K	Joback Method
tc	821.14	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	60.70	kJ/mol	418.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C64711837&Units=SI
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

chl:	Standard liquid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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