3-ETHOXYCARBONYLQUINOXALINE 1-OXIDE

Inchi: InChI=1S/C11H10N2O3/c1-2-16-11(14)9-7-13(15)10-6-4-3-5-8(10)12-9/h3-7H,2H2,1H3
InchiKey: SFQPZXAGUSTDON-UHFFFAOYSA-N
Formula: C11H10N2O3
SMILES: CCOC(=O)c1c[n+]([O-])c2ccccc2n1
Mol. weight [g/mol]: 218.21

Physical Properties

Property code	Value	Unit	Source
af	0.6102		Cheméo Relay (1.0)
hf	-125.85	kJ/mol	Cheméo Relay (1.0)
hvap	87.03	kJ/mol	Cheméo Relay (1.0)
ie	8.16	eV	Cheméo Relay (1.0)
log10ws	-2.90		Cheméo Relay (1.0)
logp	1.045		Crippen Method
mcvol	155.900	ml/mol	McGowan Method
pc	2988.26	kPa	Cheméo Relay (1.0, beta)
tb	603.17	K	Cheméo Relay (1.0)
tc	863.18	K	Cheméo Relay (1.0)
tf	420.05	K	Cheméo Relay (1.0)

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
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=C23395757&Units=SI

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