2-Methyl-3-acetyl-quinoxaline 1,4-dioxide

Inchi: InChI=1S/C11H10N2O3/c1-7-11(8(2)14)13(16)10-6-4-3-5-9(10)12(7)15/h3-6H,1-2H3
InchiKey: CUJMCPPBTUATEJ-UHFFFAOYSA-N
Formula: C11H10N2O3
SMILES: CC(=O)c1c(C)[n+]([O-])c2ccccc2[n+]1[O-]
Mol. weight [g/mol]: 218.21
CAS: 13297-17-1

Physical Properties

Property code	Value	Unit	Source
chs	-5673.90 ± 4.20	kJ/mol	NIST Webbook
hf	33.10 ± 5.00	kJ/mol	NIST Webbook
hfs	-83.90 ± 4.40	kJ/mol	NIST Webbook
hsub	117.00 ± 2.40	kJ/mol	NIST Webbook
hsub	117.00 ± 2.40	kJ/mol	NIST Webbook
log10ws	-7.47		Crippen Method
logp	0.618		Crippen Method
mcvol	155.900	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13297171&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

chs: Standard solid enthalpy of combustion
hf: Enthalpy of formation at standard conditions
hfs: Solid phase enthalpy of formation at standard conditions
hsub: Enthalpy of sublimation at standard conditions

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume