1-(4-ethylphenyl)-2,5-dihydro-1H-pyrrole-2,5-dione

Other names: 1-(4-Ethylphenyl)-2,5-dihydro-1H-pyrrole-2,5-dione
Inchi: InChI=1S/C12H11NO2/c1-2-9-3-5-10(6-4-9)13-11(14)7-8-12(13)15/h3-8H,2H2,1H3
InchiKey: FHVHFKZQDVQILM-UHFFFAOYSA-N
Formula: C12H11NO2
SMILES: CCc1ccc(N2C(=O)C=CC2=O)cc1
Mol. weight [g/mol]: 201.23

Physical Properties

Property code	Value	Unit	Source
af	0.5905		Cheméo Relay (1.0)
gf	6.05	kJ/mol	Cheméo Relay (1.0, beta)
hf	-178.12	kJ/mol	Cheméo Relay (1.0)
hvap	69.28	kJ/mol	Cheméo Relay (1.0)
ie	8.58	eV	Cheméo Relay (1.0)
log10ws	-3.41		Cheméo Relay (1.0)
logp	1.678		Crippen Method
mcvol	154.140	ml/mol	McGowan Method
pc	2892.90	kPa	Cheméo Relay (1.0, beta)
tb	575.11	K	Cheméo Relay (1.0)
tc	852.06	K	Cheméo Relay (1.0)
tf	336.91	K	Cheméo Relay (1.0)
vc	0.560	m3/kmol	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=C76620003&Units=SI

Legend

af:	Acentric Factor
gf:	Standard Gibbs free energy of formation
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
vc:	Critical Volume