1-(P-(DIMETHYLAMINO)PHENYL)-2-(2-FURYL)ETH

Other names: 1-[4-(Dimethylamino)phenyl]-2-(2-furyl)-1,2-ethanedione
Furoyl, 4-dimethylaminobenzoyl
Inchi: InChI=1S/C14H13NO3/c1-15(2)11-7-5-10(6-8-11)13(16)14(17)12-4-3-9-18-12/h3-9H,1-2
InchiKey: PHALNKSJQMXERZ-UHFFFAOYSA-N
Formula: C14H13NO3
SMILES: CN(C)c1ccc(C(=O)C(=O)c2ccco2)cc1
Mol. weight [g/mol]: 243.26

Physical Properties

Property code	Value	Unit	Source
hf	-192.67	kJ/mol	Cheméo Relay (1.0)
hvap	88.42	kJ/mol	Cheméo Relay (1.0)
ie	7.30	eV	Cheméo Relay (1.0)
log10ws	-3.29		Cheméo Relay (1.0)
logp	2.411		Crippen Method
mcvol	183.890	ml/mol	McGowan Method
rinpol	2316.00		NIST Webbook
rinpol	2316.00		NIST Webbook
tb	625.29	K	Cheméo Relay (1.0)
tf	419.16	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=C28123264&Units=SI

Legend

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point