2-ACETYLAMINO-3-AMINO-1,4-NAPHTHOQUINON

Inchi: InChI=1S/C12H10N2O3/c1-6(15)14-10-9(13)11(16)7-4-2-3-5-8(7)12(10)17/h2-5H,13H2,1
InchiKey: IZJNNHJVNPVRHJ-UHFFFAOYSA-N
Formula: C12H10N2O3
SMILES: CC(=O)NC1=C(N)C(=O)c2ccccc2C1=O
Mol. weight [g/mol]: 230.22

Physical Properties

Property code	Value	Unit	Source
hfus	26.81	kJ/mol	Joback Method
ie	8.37	eV	Cheméo Relay (1.0)
log10ws	-2.77		Cheméo Relay (1.0)
logp	0.372		Crippen Method
mcvol	165.690	ml/mol	McGowan Method
tb	626.74	K	Cheméo Relay (1.0)
tf	484.36	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	480.45	J/mol×K	842.63	Joback Method
cpg	491.52	J/mol×K	886.01	Joback Method
cpg	501.30	J/mol×K	929.39	Joback Method
cpg	509.80	J/mol×K	972.78	Joback Method
cpg	517.00	J/mol×K	1016.16	Joback Method
cpg	522.87	J/mol×K	1059.54	Joback Method
cpg	527.41	J/mol×K	1102.92	Joback Method

Sources

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=C13755969&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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