1,3-Benzodioxol, 5-(acetylaminomethyl)

Inchi: InChI=1S/C10H11NO3/c1-7(12)11-5-8-2-3-9-10(4-8)14-6-13-9/h2-4H,5-6H2,1H3,(H,11,1
InchiKey: YFWYIWVJRPDXQD-UHFFFAOYSA-N
Formula: C10H11NO3
SMILES: CC(=O)NCc1ccc2c(c1)OCO2
Mol. weight [g/mol]: 193.20

Physical Properties

Property code	Value	Unit	Source
hfus	34.64	kJ/mol	Joback Method
hvap	84.81	kJ/mol	Cheméo Relay (1.0)
ie	8.10	eV	Cheméo Relay (1.0)
log10ws	-2.08		Cheméo Relay (1.0)
logp	1.051		Crippen Method
mcvol	140.430	ml/mol	McGowan Method
rinpol	1940.00		NIST Webbook
rinpol	1940.00		NIST Webbook
tb	588.16	K	Cheméo Relay (1.0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	-2.68990e+01
Coeff. B	9.75520e-01
Coeff. C	-6.95020e-04
Coeff. D	1.95060e-07
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Sources

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=R408856&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion 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

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