P-ACETAMIDOPHENYL ACETATE

Other names: p-acetoxy-acetanilide
Inchi: InChI=1S/C10H11NO3/c1-7(12)11-9-3-5-10(6-4-9)14-8(2)13/h3-6H,1-2H3,(H,11,12)
InchiKey: UJAOSPFULOFZRR-UHFFFAOYSA-N
Formula: C10H11NO3
SMILES: CC(=O)Nc1ccc(OC(C)=O)cc1
Mol. weight [g/mol]: 193.20

Physical Properties

Property code	Value	Unit	Source
hf	-484.69	kJ/mol	Cheméo Relay (1.0)
hfus	24.79	kJ/mol	Joback Method
hvap	80.05	kJ/mol	Cheméo Relay (1.0)
ie	7.81	eV	Cheméo Relay (1.0)
log10ws	-1.91		Aqueous Solubility Prediction Method
logp	1.570		Crippen Method
mcvol	146.990	ml/mol	McGowan Method
tb	575.66	K	Cheméo Relay (1.0)
tf	396.49	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	362.17	J/mol×K	640.19	Joback Method
cpg	374.16	J/mol×K	676.98	Joback Method
cpg	385.36	J/mol×K	713.78	Joback Method
cpg	395.79	J/mol×K	750.57	Joback Method
cpg	405.45	J/mol×K	787.37	Joback Method
cpg	414.37	J/mol×K	824.16	Joback Method
cpg	422.55	J/mol×K	860.95	Joback Method

Sources

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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2623338&Units=SI

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point