

2-Acetamido-4-methylphenyl acetate

Other names:	2-N-Acetylamino-4-methylphenol acetate
Inchi:	InChI=1S/C11H13NO3/c1-7-4-5-11(15-9(3)14)10(6-7)12-8(2)13/h4-6H,1-3H3,(H,12,13)
InchiKey:	GPJFMEZBKSINFK-UHFFFAOYSA-N
Formula:	C11H13NO3
SMILES:	CC(=O)Nc1cc(C)ccc1OC(C)=O
Mol. weight [g/mol]:	207.23

Physical Properties

Property code	Value	Unit	Source
gf	-138.56	kJ/mol	Joback Method
hf	-360.69	kJ/mol	Joback Method
hfus	26.99	kJ/mol	Joback Method
hvap	66.02	kJ/mol	Joback Method
log10ws	-2.46		Crippen Method
logp	1.879		Crippen Method
mcvol	161.080	ml/mol	McGowan Method
pc	2918.68	kPa	Joback Method
rinpol	1703.00		NIST Webbook
tb	668.05	K	Joback Method
tc	885.88	K	Joback Method
tf	439.94	K	Joback Method
vc	0.609	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	410.21	J/molxK	668.05	Joback Method
cpg	422.70	J/molxK	704.36	Joback Method
cpg	434.40	J/molxK	740.66	Joback Method
cpg	445.32	J/molxK	776.97	Joback Method
cpg	455.45	J/molxK	813.27	Joback Method
cpg	464.82	J/molxK	849.58	Joback Method
cpg	473.43	J/molxK	885.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373469&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvp:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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