Acetamide, N-(4-methoxyphenyl)-2-acetoxy-

Inchi: InChI=1S/C11H13NO4/c1-8(13)16-7-11(14)12-9-3-5-10(15-2)6-4-9/h3-6H,7H2,1-2H3,(H,
InchiKey: CLMGQGQQLDVOCU-UHFFFAOYSA-N
Formula: C11H13NO4
SMILES: COc1ccc(NC(=O)COC(C)=O)cc1
Mol. weight [g/mol]: 223.23

Physical Properties

Property code	Value	Unit	Source
gf	-233.93	kJ/mol	Joback Method
hf	-481.44	kJ/mol	Joback Method
hfus	28.57	kJ/mol	Joback Method
hvap	67.77	kJ/mol	Joback Method
log10ws	-1.49		Crippen Method
logp	1.197		Crippen Method
mcvol	166.950	ml/mol	McGowan Method
pc	2912.39	kPa	Joback Method
rinpol	1901.00		NIST Webbook
tb	685.49	K	Joback Method
tc	900.03	K	Joback Method
tf	449.65	K	Joback Method
vc	0.626	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	435.99	J/mol×K	685.49	Joback Method
cpg	448.41	J/mol×K	721.25	Joback Method
cpg	460.02	J/mol×K	757.00	Joback Method
cpg	470.80	J/mol×K	792.76	Joback Method
cpg	480.77	J/mol×K	828.52	Joback Method
cpg	489.91	J/mol×K	864.28	Joback Method
cpg	498.24	J/mol×K	900.03	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307093&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hvap:	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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume