

Ethanone, 2-(acetyloxy)-1-phenyl-

Other names:	Acetophenone, 2-hydroxy-, acetate «omega»-Acetoxyacetophenone Phenacyl acetate 2-Hydroxyacetophenoneacetate 2-Acetoxy-1-phenylethanone NSC 9837
Inchi:	InChI=1S/C10H10O3/c1-8(11)13-7-10(12)9-5-3-2-4-6-9/h2-6H,7H2,1H3
InchiKey:	BGAXCPSNMHVHJC-UHFFFAOYSA-N
Formula:	C10H10O3
SMILES:	CC(=O)OCC(=O)c1ccccc1
Mol. weight [g/mol]:	178.18
CAS:	2243-35-8

Physical Properties

Property code	Value	Unit	Source
gf	-217.11	kJ/mol	Joback Method
hf	-370.58	kJ/mol	Joback Method
hfus	20.08	kJ/mol	Joback Method
hvap	56.03	kJ/mol	Joback Method
log10ws	-1.83		Crippen Method
logp	1.432		Crippen Method
mcvol	137.010	ml/mol	McGowan Method
pc	3310.55	kPa	Joback Method
tb	585.04	K	Joback Method
tc	805.88	K	Joback Method
tf	350.97	K	Joback Method
vc	0.517	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	316.40	J/mol×K	585.04	Joback Method
cpg	370.44	J/mol×K	769.07	Joback Method
cpg	361.13	J/mol×K	732.27	Joback Method

cpg	351.09	J/molxK	695.46	Joback Method
cpg	340.30	J/molxK	658.65	Joback Method
cpg	328.74	J/molxK	621.85	Joback Method
cpg	379.03	J/molxK	805.88	Joback Method
dvisc	0.0002309	Paxs	585.04	Joback Method
dvisc	0.0002912	Paxs	546.03	Joback Method
dvisc	0.0003805	Paxs	507.02	Joback Method
dvisc	0.0005201	Paxs	468.00	Joback Method
dvisc	0.0007523	Paxs	428.99	Joback Method
dvisc	0.0011717	Paxs	389.98	Joback Method
dvisc	0.0020137	Paxs	350.97	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2243358&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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