

2-Benzoyloxyacetophenone

Other names:	2-Acetylphenyl benzoate o-Benzoyloxyacetophenone o-Acetylphenyl benzoate Ethanone, 1-(2-(benzoyloxy)phenyl)- Acetophenone, 2'-hydroxy-, benzoate Benzoic acid, 2-acetylphenyl ester Benzoic acid, o-acetylphenyl ester-
Inchi:	InChI=1S/C15H12O3/c1-11(16)13-9-5-6-10-14(13)18-15(17)12-7-3-2-4-8-12/h2-10H,1H3
InchiKey:	UEVPPUDQJRWOLT-UHFFFAOYSA-N
Formula:	C15H12O3
SMILES:	CC(=O)c1ccccc1OC(=O)c1ccccc1
Mol. weight [g/mol]:	240.25
CAS:	4010-33-7

Physical Properties

Property code	Value	Unit	Source
gf	-72.23	kJ/mol	Joback Method
hf	-248.72	kJ/mol	Joback Method
hfus	26.68	kJ/mol	Joback Method
hvap	70.10	kJ/mol	Joback Method
log10ws	-4.22		Crippen Method
logp	3.108		Crippen Method
mcvol	183.700	ml/mol	McGowan Method
pc	2764.26	kPa	Joback Method
tb	731.10	K	Joback Method
tc	975.09	K	Joback Method
tf	446.26	K	Joback Method
vc	0.690	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	480.02	J/mol×K	731.10	Joback Method
cpg	493.68	J/mol×K	771.76	Joback Method

cpg	506.15	J/mol×K	812.43	Joback Method
cpg	517.48	J/mol×K	853.09	Joback Method
cpg	527.71	J/mol×K	893.76	Joback Method
cpg	536.90	J/mol×K	934.42	Joback Method
cpg	545.09	J/mol×K	975.09	Joback Method
dvisc	0.0010757	Pa×s	446.26	Joback Method
dvisc	0.0006479	Pa×s	493.73	Joback Method
dvisc	0.0004265	Pa×s	541.21	Joback Method
dvisc	0.0003004	Pa×s	588.68	Joback Method
dvisc	0.0002229	Pa×s	636.15	Joback Method
dvisc	0.0001724	Pa×s	683.63	Joback Method
dvisc	0.0001379	Pa×s	731.10	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=C4010337&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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