

3-Butenenitrile, 2-(benzoyloxy)-4-phenyl-

Other names:	3-Butenenitrile, 2-hydroxy-4-phenyl-, benzoate (ester) 2-Benzoyloxy-4-phenyl-3-butenenitrile Benzoic acid, alpha-cyanocinnamyl ester 1-Cyano-3-phenyl-2-propenyl benzoate
Inchi:	InChI=1S/C17H13NO2/c18-13-16(12-11-14-7-3-1-4-8-14)20-17(19)15-9-5-2-6-10-15/h1-
InchiKey:	HEHFCYOFVZHSGV-VAWYXSNFSA-N
Formula:	C17H13NO2
SMILES:	N#CC(C=Cc1ccccc1)OC(=O)c1ccccc1
Mol. weight [g/mol]:	263.29
CAS:	1591-17-9

Physical Properties

Property code	Value	Unit	Source
gf	294.12	kJ/mol	Joback Method
hf	110.87	kJ/mol	Joback Method
hfus	28.84	kJ/mol	Joback Method
hvap	77.19	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	3.449		Crippen Method
mcvol	207.390	ml/mol	McGowan Method
pc	2252.53	kPa	Joback Method
tb	823.81	K	Joback Method
tc	1075.41	K	Joback Method
tf	451.26	K	Joback Method
vc	0.795	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	568.26	J/molxK	823.81	Joback Method
cpg	580.67	J/molxK	865.74	Joback Method
cpg	591.95	J/molxK	907.68	Joback Method
cpg	602.19	J/molxK	949.61	Joback Method
cpg	611.51	J/molxK	991.54	Joback Method

cpg	619.98	J/mol×K	1033.47	Joback Method
cpg	627.71	J/mol×K	1075.41	Joback Method

Sources

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=C1591179&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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