Benorilate

Other names:	Benzoic acid, 2-(acetyloxy)-, 4-(acetylamino)phenyl ester
	Salicylic acid, acetate, ester with 4'-hydroxyacetanilide
	4'-(Acetamido)phenyl-2-acetoxybenzoate
	p-Acetamidophenyl acetylsalicylate
	2-Acetoxy-4'-(acetamino)phenylbenzoate
	p-N-Acetylaminophenylacetylsalicylate
	2-(Acetyloxy)benzoic acid 4-(acetylamino)phenyl ester
	Aspirin acetaminophen ester
	Benoral
	Benorilato
	Benortan
	Benorylate
	Fenasparate
	Salipran
	TO 125
	WIN 11450
	4-Acetamidophenyl salicylate acetate
	Fenasprate
	Quinexin
Inchi:	InChI=1S/C17H15NO5/c1-11(19)18-13-7-9-14(10-8-13)23-17(21)15-5-3-4-6-16(15)22-12
InchiKey:	FEJKLNWAOXSSNR-UHFFFAOYSA-N
Formula:	C17H15NO5
SMILES:	CC(=O)Nc1ccc(OC(=O)c2ccccc2OC(C)=O)cc1
Mol. weight [g/mol]:	313.30
CAS:	5003-48-5

Physical Properties

Property code	Value	Unit	Source
gf	-209.55	kJ/mol	Joback Method
hf	-492.80	kJ/mol	Joback Method
hfus	39.36	kJ/mol	Joback Method
hvap	90.81	kJ/mol	Joback Method
log10ws	-4.07		Crippen Method
logp	2.789		Crippen Method
mcvol	229.300	ml/mol	McGowan Method
pc	2379.54	kPa	Joback Method
tb	908.30	K	Joback Method

tc	1145.45	K	Joback Method
tf	606.14	K	Joback Method
vc	0.861	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	671.83	J/mol×K	908.30	Joback Method
cpg	682.32	J/mol×K	947.82	Joback Method
cpg	691.51	J/mol×K	987.35	Joback Method
cpg	699.45	J/mol×K	1026.87	Joback Method
cpg	706.15	J/mol×K	1066.40	Joback Method
cpg	711.63	J/mol×K	1105.92	Joback Method
cpg	715.92	J/mol×K	1145.45	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5003485&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
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