Benzoic acid, 2-[[[4-[(acetylamino)sulfonyl]phenyl]amino]carbo

Other names:	2-[[4-(acetylsulfamoyl)phenyl]carbamoyl]benzoic acid
	4'-(Acetylsulfamoyl)phthalanilic acid
	4'-(Acetylsulfamyl)phthalanilic acid
	Enterocid
	Enterosulfamid
	Enterosulfon
	Enterosulphamid
	Ftalicetimida
	Kalacet
	N-(4-(acetylsulphamoyl)phenyl)phthalamic acid
	N-(o-Carboxybenzoyl)sulfacetamide
	N1-Acetyl-N4-phthalylsulfanilamide
	NSC 163977
	Phthalanilic acid, 4'-(acetylsulfamoyl)-
	Phthaloylsulfacetamide
	Phthalylsulfacetamide
	Phthalylsulfacetimide
	Phthalylsulphacetamide
	Phthalylthioacetamide
	Rabalan
	Sterathal
	Sulphalyl
	TSC-80
	TSC-80 Medicated
	Talasulfa
	Talecid
	Talicetimida
	Talsigel
	Talsutin
	Tamid
	Thalajen
	Thalamyd
	Thalisul
	Thalocid
Inchi:	InChI=1S/C16H14N2O6S/c1-10(19)18-25(23,24)12-8-6-11(7-9-12)17-15(20)13-4-2-3-5-1
InchiKey:	SNWQKAWITMVCQW-UHFFFAOYSA-N
Formula:	C16H14N2O6S
SMILES:	CC(=O)NS(=O)(=O)c1ccc(NC(=O)c2ccccc2C(=O)O)cc1
Mol. weight [g/mol]:	362.36
CAS:	131-69-1

Physical Properties

Property code	Value	Unit	Source
gf	-523.94	kJ/mol	Joback Method
hf	-759.83	kJ/mol	Joback Method
hfus	54.96	kJ/mol	Joback Method
hvap	125.51	kJ/mol	Joback Method
log10ws	-2.52		Aqueous Solubility Prediction Method
logp	1.462		Crippen Method
mcvol	247.410	ml/mol	McGowan Method
pc	3628.97	kPa	Joback Method
tb	1030.71	K	Joback Method
tc	1267.10	K	Joback Method
tf	702.45	K	Joback Method
vc	0.949	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	735.65	J/mol×K	1030.71	Joback Method
cpg	741.28	J/mol×K	1070.11	Joback Method
cpg	745.68	J/mol×K	1109.51	Joback Method
cpg	748.92	J/mol×K	1148.90	Joback Method
cpg	751.02	J/mol×K	1188.30	Joback Method
cpg	752.03	J/mol×K	1227.70	Joback Method
cpg	752.01	J/mol×K	1267.10	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C131691&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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