3-ACETAMIDO-2,4,6-TRIIODOBENZOIC ACID

Other names:	Acetrizoic acid
	3-Acetamino-2,4,6-triiodobenzoic acid
	Benzoic acid, 3-(acetylamino)-2,4,6-triiodo-
	Benzoic acid, 3-acetamido-2,4,6-triiodo-
	3-(Acetylamino)-2,4,6-triiodobenzoic acid
	Acido 3-acetilamino-2,4,6-triiodobenzoico
Inchi:	InChI=1S/C9H6I3NO3/c1-3(14)13-8-5(11)2-4(10)6(7(8)12)9(15)16/h2H,1H3,(H,13,14)(H,
InchiKey:	GNOGSFBXBWBTIG-UHFFFAOYSA-N
Formula:	C9H6I3NO3
SMILES:	CC(=O)Nc1c(I)cc(I)c(C(=O)O)c1I
Mol. weight [g/mol]:	556.86

Physical Properties

Property code	Value	Unit	Source
hfus	37.15	kJ/mol	Joback Method
log10ws	-3.79		Cheméo Relay (1.0)
logp	3.157		Crippen Method
mcvol	210.360	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	411.90	J/mol×K	981.43	Joback Method
cpg	417.14	J/mol×K	1027.24	Joback Method
cpg	422.08	J/mol×K	1073.06	Joback Method
cpg	426.80	J/mol×K	1118.87	Joback Method
cpg	431.39	J/mol×K	1164.69	Joback Method
cpg	435.92	J/mol×K	1210.50	Joback Method
cpg	440.48	J/mol×K	1256.31	Joback Method

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C85369&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume