

3-Acetamido-2,4,6-triiodobenzoic acid

Other names:	Acetrizic 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
CAS:	85-36-9

Physical Properties

Property code	Value	Unit	Source
gf	-32.12	kJ/mol	Joback Method
hf	-131.75	kJ/mol	Joback Method
hfus	37.15	kJ/mol	Joback Method
hvap	105.28	kJ/mol	Joback Method
log10ws	-5.18		Crippen Method
logp	3.157		Crippen Method
mcvol	210.360	ml/mol	McGowan Method
pc	3690.97	kPa	Joback Method
tb	981.43	K	Joback Method
tc	1256.31	K	Joback Method
tf	655.21	K	Joback Method
vc	0.761	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	411.90	J/molxK	981.43	Joback Method
cpg	417.14	J/molxK	1027.24	Joback Method
cpg	422.08	J/molxK	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

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=C85369&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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