Iopanoic Acid

Other names:	(+) 3-[3-(Amino-2,4,6-triiodophenyl]-2-ethylpropanoic acid (iopanoic acid)
	(.+/-.)-Iopanoic acid
	2-(3-Amino-2,4,6-triiodobenzyl)butyric acid
	2-Ethyl-3-(3-amino-2,4,6-triiodophenyl)propionic acid
	3-(3-Amino-2,4,6-triiodophenyl)-2-ethylpropanoic acid
	3-Amino-«alpha»-ethyl-2,4,6-triiodobenzenepropanoic acid
	3-Amino-«alpha»-ethyl-2,4,6-triiodohydrocinnamic acid
	3-Amino-Â«alphaÂ»-ethyl-2,4,6-triiodobenzenepropanoic acid
	3-Amino-Â«alphaÂ»-ethyl-2,4,6-triiodohydrocinnamic acid
	Benzenepropanoic acid, 3-amino-«alpha»-ethyl-2,4,6-triiodo-
	Benzenepropanoic acid, 3-amino-«alpha»-ethyl-2,4,6-triiodo-, (.+/-.)-
	Benzenepropanoic acid, 3-amino-Â«alphaÂ»-ethyl-2,4,6-triiodo-
	Benzenepropanoic acid, 3-amino-Â«alphaÂ»-ethyl-2,4,6-triiodo-, (.+/-.)-
	Bilijodon
	Choladine
	Cholevid
	Cistobil
	Colepax
	Copanoic
	Hydrocinnamic acid, 3-amino-«alpha»-ethyl-2,4,6-triiodo-
	Hydrocinnamic acid, 3-amino-Â«alphaÂ»-ethyl-2,4,6-triiodo-
	Iodopanic acid
	Iodopanoic acid
	Iopagnost
	Iopanoicum
	Jopagnost
	Jopanoic acid
	NSC 41706
	Polognost
	Telepaque
	Teletrast
	«alpha»-Ethyl-«beta»-(3-amino-2,4,6-triiodophenyl)propionic acid
	«beta»-(3-Amino-2,4,6-triiodophenyl)-«alpha»-ethylpropionic acid
	Â«alphaÂ»-Ethyl-Â«betaÂ»-(3-amino-2,4,6-triiodophenyl)propionic acid
	Â«betaÂ»-(3-Amino-2,4,6-triiodophenyl)-Â«alphaÂ»-ethylpropionic acid
Inchi:	InChI=1S/C11H12I3NO2/c1-2-5(11(16)17)3-6-7(12)4-8(13)10(15)9(6)14/h4-5H,2-3,15H2
InchiKey:	OIRFJRBSRORBCM-UHFFFAOYSA-N
Formula:	C11H12I3NO2
SMILES:	CCC(Cc1c(I)cc(I)c(N)c1I)C(=O)O
Mol. weight [g/mol]:	570.93

CAS: 96-83-3

Physical Properties

Property code	Value	Unit	Source
gf	88.26	kJ/mol	Joback Method
hf	-85.41	kJ/mol	Joback Method
hfus	37.31	kJ/mol	Joback Method
hvap	106.80	kJ/mol	Joback Method
log10ws	-5.48		Aqueous Solubility Prediction Method
logp	3.736		Crippen Method
mcvol	236.970	ml/mol	McGowan Method
pc	2925.00	kPa	Joback Method
tb	995.24	K	Joback Method
tc	1267.45	K	Joback Method
tf	428.35	K	Aqueous Solubility Prediction Method
vc	0.856	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	527.03	J/mol×K	995.24	Joback Method
cpg	534.67	J/mol×K	1040.61	Joback Method
cpg	541.95	J/mol×K	1085.98	Joback Method
cpg	548.95	J/mol×K	1131.35	Joback Method
cpg	555.79	J/mol×K	1176.71	Joback Method
cpg	562.56	J/mol×K	1222.08	Joback Method
cpg	569.36	J/mol×K	1267.45	Joback Method
hfust	27.70	kJ/mol	427.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C96833&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
hfust:	Enthalpy of fusion at a given temperature
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