

3-Iodo-5-nitrobenzoic acid

Inchi:	InChI=1S/C7H4INO4/c8-5-1-4(7(10)11)2-6(3-5)9(12)13/h1-3H,(H,10,11)
InchiKey:	GFGURBBHVJTXDU-UHFFFAOYSA-N
Formula:	C7H4INO4
SMILES:	O=C(O)c1cc(I)cc([N+](=O)[O-])c1
Mol. weight [g/mol]:	293.02
CAS:	6313-17-3

Physical Properties

Property code	Value	Unit	Source
gf	-70.86	kJ/mol	Joback Method
hf	-172.92	kJ/mol	Joback Method
hfus	28.60	kJ/mol	Joback Method
hvap	84.16	kJ/mol	Joback Method
log10ws	-3.33		Crippen Method
logp	1.898		Crippen Method
mcvol	136.410	ml/mol	McGowan Method
pc	4795.85	kPa	Joback Method
tb	787.23	K	Joback Method
tc	1045.32	K	Joback Method
tf	532.53	K	Joback Method
vc	0.514	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	294.45	J/molxK	787.23	Joback Method
cpg	300.44	J/molxK	830.24	Joback Method
cpg	305.86	J/molxK	873.26	Joback Method
cpg	310.74	J/molxK	916.27	Joback Method
cpg	315.16	J/molxK	959.29	Joback Method
cpg	319.15	J/molxK	1002.30	Joback Method
cpg	322.78	J/molxK	1045.32	Joback Method

Sources

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=C6313173&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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