2-Iodo-4-methyl-6-nitrophenol

Inchi: InChI=1S/C7H6INO3/c1-4-2-5(8)7(10)6(3-4)9(11)12/h2-3,10H,1H3
InchiKey: ZGSKNXKQYFZYAW-UHFFFAOYSA-N
Formula: C7H6INO3
SMILES: Cc1cc(I)c(O)c([N+](=O)[O-])c1
Mol. weight [g/mol]: 279.03
CAS: 69492-91-7

Physical Properties

Property code	Value	Unit	Source
gf	40.26	kJ/mol	Joback Method
hf	-85.42	kJ/mol	Joback Method
hfus	28.70	kJ/mol	Joback Method
hvap	73.75	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	2.213		Crippen Method
mcvol	134.840	ml/mol	McGowan Method
pc	4756.24	kPa	Joback Method
tb	721.80	K	Joback Method
tc	1010.62	K	Joback Method
tf	533.50	K	Joback Method
vc	0.456	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	292.11	J/mol×K	721.80	Joback Method
cpg	300.09	J/mol×K	769.94	Joback Method
cpg	307.54	J/mol×K	818.07	Joback Method
cpg	314.61	J/mol×K	866.21	Joback Method
cpg	321.48	J/mol×K	914.35	Joback Method
cpg	328.30	J/mol×K	962.48	Joback Method
cpg	335.23	J/mol×K	1010.62	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=C69492917&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