Anthranilic acid, n-(o-nitrophenyl)-

Inchi: InChI=1S/C13H10N2O4/c16-13(17)9-5-1-2-6-10(9)14-11-7-3-4-8-12(11)15(18)19/h1-8,14
InchiKey: FJNZXTAFUISVCI-UHFFFAOYSA-N
Formula: C13H10N2O4
SMILES: O=C(O)c1ccccc1Nc1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]: 258.23
CAS: 5933-35-7

Physical Properties

Property code	Value	Unit	Source
gf	123.34	kJ/mol	Joback Method
hf	-83.63	kJ/mol	Joback Method
hfus	38.88	kJ/mol	Joback Method
hvap	96.86	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	3.037		Crippen Method
mcvol	181.350	ml/mol	McGowan Method
pc	3655.35	kPa	Joback Method
tb	908.22	K	Joback Method
tc	1154.92	K	Joback Method
tf	621.17	K	Joback Method
vc	0.690	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	520.07	J/mol×K	908.22	Joback Method
cpg	528.48	J/mol×K	949.34	Joback Method
cpg	536.05	J/mol×K	990.45	Joback Method
cpg	542.84	J/mol×K	1031.57	Joback Method
cpg	548.94	J/mol×K	1072.69	Joback Method
cpg	554.41	J/mol×K	1113.80	Joback Method
cpg	559.32	J/mol×K	1154.92	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=C5933357&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