Benzoic acid, o-nitropheyl ester

Inchi: InChI=1S/C13H9NO4/c15-13(10-6-2-1-3-7-10)18-12-9-5-4-8-11(12)14(16)17/h1-9H
InchiKey: PNBOBRKDXRJMTL-UHFFFAOYSA-N
Formula: C13H9NO4
SMILES: O=C(Oc1ccccc1[N+](=O)[O-])c1ccccc1
Mol. weight [g/mol]: 243.21
CAS: 1523-12-2

Physical Properties

Property code	Value	Unit	Source
gf	75.40	kJ/mol	Joback Method
hf	-105.62	kJ/mol	Joback Method
hfus	31.27	kJ/mol	Joback Method
hvap	75.49	kJ/mol	Joback Method
log10ws	-4.21		Crippen Method
logp	2.814		Crippen Method
mcvol	171.370	ml/mol	McGowan Method
pc	3224.64	kPa	Joback Method
tb	783.31	K	Joback Method
tc	1050.92	K	Joback Method
tf	517.40	K	Joback Method
vc	0.653	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	457.81	J/mol×K	783.31	Joback Method
cpg	469.55	J/mol×K	827.91	Joback Method
cpg	480.03	J/mol×K	872.51	Joback Method
cpg	489.33	J/mol×K	917.11	Joback Method
cpg	497.50	J/mol×K	961.72	Joback Method
cpg	504.62	J/mol×K	1006.32	Joback Method
cpg	510.75	J/mol×K	1050.92	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=C1523122&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