3-Bromobenzoic acid, 4-nitrophenyl ester

Inchi: InChI=1S/C13H8BrNO4/c14-10-3-1-2-9(8-10)13(16)19-12-6-4-11(5-7-12)15(17)18/h1-8H
InchiKey: SDTSMRAQTBFFQM-UHFFFAOYSA-N
Formula: C13H8BrNO4
SMILES: O=C(Oc1ccc([N+](=O)[O-])cc1)c1cccc(Br)c1
Mol. weight [g/mol]: 322.11

Physical Properties

Property code	Value	Unit	Source
gf	80.09	kJ/mol	Joback Method
hf	-90.76	kJ/mol	Joback Method
hfus	36.16	kJ/mol	Joback Method
hvap	82.59	kJ/mol	Joback Method
log10ws	-5.37		Crippen Method
logp	3.576		Crippen Method
mcvol	188.870	ml/mol	McGowan Method
pc	3431.89	kPa	Joback Method
rinpol	2368.00		NIST Webbook
rinpol	2368.00		NIST Webbook
tb	854.45	K	Joback Method
tc	1131.19	K	Joback Method
tf	589.72	K	Joback Method
vc	0.716	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	482.78	J/mol×K	854.45	Joback Method
cpg	492.50	J/mol×K	900.57	Joback Method
cpg	501.09	J/mol×K	946.70	Joback Method
cpg	508.62	J/mol×K	992.82	Joback Method
cpg	515.17	J/mol×K	1038.95	Joback Method
cpg	520.81	J/mol×K	1085.07	Joback Method
cpg	525.64	J/mol×K	1131.19	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=U307554&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume