(Z)-3-(o-Bromophenylamino)-2-nitrocrotonic acid methyl ester

Inchi: InChI=1S/C11H11BrN2O4/c1-7(10(14(16)17)11(15)18-2)13-9-6-4-3-5-8(9)12/h3-6,13H,1

InchiKey: YTXNBNGNYHWPFP-YFHOEESVSA-N

Formula: C11H11BrN2O4

SMILES: COC(=O)C(=C(C)Nc1ccccc1Br)[N+](=O)[O-]

Mol. weight [g/mol]: 315.12

CAS: 127727-83-7

Physical Properties

Property code	Value	Unit	Source
gf	112.98	kJ/mol	Joback Method
hf	-123.43	kJ/mol	Joback Method
hfus	40.01	kJ/mol	Joback Method
hvap	81.75	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	2.542		Crippen Method
mcvol	190.130	ml/mol	McGowan Method
pc	3243.03	kPa	Joback Method
tb	831.12	K	Joback Method
tc	1086.81	K	Joback Method
tf	547.90	K	Joback Method
vc	0.729	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	498.05	J/mol×K	831.12	Joback Method
cpg	508.32	J/mol×K	873.74	Joback Method
cpg	517.71	J/mol×K	916.35	Joback Method
cpg	526.29	J/mol×K	958.97	Joback Method
cpg	534.13	J/mol×K	1001.58	Joback Method
cpg	541.32	J/mol×K	1044.20	Joback Method
cpg	547.94	J/mol×K	1086.81	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C127727837&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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