(Z)-3-(p-Chlorophenylamino)-2-nitrocrotonic methyl ester

Inchi: InChI=1S/C11H11ClN2O4/c1-7(10(14(16)17)11(15)18-2)13-9-5-3-8(12)4-6-9/h3-6,13H,1

InchiKey: BNXNUQUDLCHRTM-YFHOEESVSA-N

Formula: C11H11ClN2O4

SMILES: COC(=O)C(=C(C)Nc1ccc(Cl)cc1)[N+](=O)[O-]

Mol. weight [g/mol]: 270.67

CAS: 116343-84-1

Physical Properties

Property code	Value	Unit	Source
gf	86.73	kJ/mol	Joback Method
hf	-165.50	kJ/mol	Joback Method
hfus	38.92	kJ/mol	Joback Method
hvap	79.70	kJ/mol	Joback Method
log10ws	-3.63		Crippen Method
logp	2.433		Crippen Method
mcvol	184.870	ml/mol	McGowan Method
pc	2884.30	kPa	Joback Method
tb	802.39	K	Joback Method
tc	1051.01	K	Joback Method
tf	518.02	K	Joback Method
vc	0.716	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	489.95	J/mol×K	802.39	Joback Method
cpg	500.65	J/mol×K	843.83	Joback Method
cpg	510.41	J/mol×K	885.26	Joback Method
cpg	519.29	J/mol×K	926.70	Joback Method
cpg	527.36	J/mol×K	968.14	Joback Method
cpg	534.68	J/mol×K	1009.57	Joback Method
cpg	541.31	J/mol×K	1051.01	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116343841&Units=SI

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