(Z) Methyl 2-nitro-3-phenylpropenoate

Inchi: InChI=1S/C10H9NO4/c1-15-10(12)7-9(11(13)14)8-5-3-2-4-6-8/h2-7H,1H3/b9-7-
InchiKey: ZRJCWSPYKILXGU-CLFYSBASSA-N
Formula: C10H9NO4
SMILES: COC(=O)C=C(c1ccccc1)[N+](=O)[O-]
Mol. weight [g/mol]: 207.18
CAS: 42251-12-7

Physical Properties

Property code	Value	Unit	Source
gf	19.03	kJ/mol	Joback Method
hf	-161.33	kJ/mol	Joback Method
hfus	28.74	kJ/mol	Joback Method
hvap	65.91	kJ/mol	Joback Method
log10ws	-2.57		Crippen Method
logp	1.477		Crippen Method
mcvol	148.560	ml/mol	McGowan Method
pc	3333.53	kPa	Joback Method
tb	687.05	K	Joback Method
tc	937.69	K	Joback Method
tf	425.61	K	Joback Method
vc	0.575	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.96	J/mol×K	687.05	Joback Method
cpg	384.71	J/mol×K	728.82	Joback Method
cpg	395.47	J/mol×K	770.60	Joback Method
cpg	405.30	J/mol×K	812.37	Joback Method
cpg	414.26	J/mol×K	854.14	Joback Method
cpg	422.41	J/mol×K	895.92	Joback Method
cpg	429.82	J/mol×K	937.69	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C42251127&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