Methyl (3-nitrophenyl)acetate

Inchi: InChI=1S/C9H9NO4/c1-14-9(11)6-7-3-2-4-8(5-7)10(12)13/h2-5H,6H2,1H3
InchiKey: BFGYITRIATVARH-UHFFFAOYSA-N
Formula: C9H9NO4
SMILES: COC(=O)Cc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 195.17

Physical Properties

Property code	Value	Unit	Source
gf	-70.69	kJ/mol	Joback Method
hf	-259.59	kJ/mol	Joback Method
hfus	26.87	kJ/mol	Joback Method
hvap	64.31	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	1.310		Crippen Method
mcvol	138.770	ml/mol	McGowan Method
pc	3427.87	kPa	Joback Method
rinpol	1613.00		NIST Webbook
tb	665.11	K	Joback Method
tc	907.46	K	Joback Method
tf	445.90	K	Joback Method
vc	0.537	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	345.96	J/mol×K	665.11	Joback Method
cpg	357.42	J/mol×K	705.50	Joback Method
cpg	367.99	J/mol×K	745.89	Joback Method
cpg	377.72	J/mol×K	786.28	Joback Method
cpg	386.61	J/mol×K	826.67	Joback Method
cpg	394.70	J/mol×K	867.07	Joback Method
cpg	401.99	J/mol×K	907.46	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R190080&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume