(2-NITROPHENYL)ACETIC ACID, METHYL ESTER

Other names: Methyl (2-nitrophenyl)acetate
Inchi: InChI=1S/C9H9NO4/c1-14-9(11)6-7-4-2-3-5-8(7)10(12)13/h2-5H,6H2,1H3
InchiKey: SWMFAAPTSMVULA-UHFFFAOYSA-N
Formula: C9H9NO4
SMILES: COC(=O)Cc1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]: 195.17

Physical Properties

Property code	Value	Unit	Source
hf	-277.30	kJ/mol	Cheméo Relay (1.0)
hfus	26.87	kJ/mol	Joback Method
hvap	79.39	kJ/mol	Cheméo Relay (1.0)
ie	9.32	eV	Cheméo Relay (1.0)
log10ws	-2.30		Cheméo Relay (1.0)
logp	1.310		Crippen Method
mcvol	138.770	ml/mol	McGowan Method
tb	555.99	K	Cheméo Relay (1.0)
tf	302.31	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C30095988&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point