2-NITROPHENYL ACETATE

Inchi: InChI=1S/C8H7NO4/c1-6(10)13-8-5-3-2-4-7(8)9(11)12/h2-5H,1H3
InchiKey: MRCKRGSNLOHYRA-UHFFFAOYSA-N
Formula: C8H7NO4
SMILES: CC(=O)Oc1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]: 181.15

Physical Properties

Property code	Value	Unit	Source
hf	-278.48	kJ/mol	Cheméo Relay (1.0)
hfus	24.28	kJ/mol	Joback Method
hvap	72.39	kJ/mol	Cheméo Relay (1.0)
ie	9.14	eV	Cheméo Relay (1.0)
log10ws	-2.38		Cheméo Relay (1.0)
logp	1.520		Crippen Method
mcvol	124.680	ml/mol	McGowan Method
tb	533.44	K	Cheméo Relay (1.0)
tf	308.67	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.26	J/mol×K	642.23	Joback Method
cpg	308.88	J/mol×K	683.52	Joback Method
cpg	318.68	J/mol×K	724.81	Joback Method
cpg	327.67	J/mol×K	766.10	Joback Method
cpg	335.88	J/mol×K	807.39	Joback Method
cpg	343.31	J/mol×K	848.68	Joback Method
cpg	349.99	J/mol×K	889.97	Joback Method
hvapt	71.10	kJ/mol	449.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	414.20	K	1.50	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C610695&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

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
hvapt:	Enthalpy of vaporization at a given temperature
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
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point