3-Nitrobenzeneacetyl chloride

Inchi: InChI=1S/C8H6ClNO3/c9-5-8(11)6-2-1-3-7(4-6)10(12)13/h1-4H,5H2
InchiKey: LBHUVZXFCGZYDL-UHFFFAOYSA-N
Formula: C8H6ClNO3
SMILES: O=C(CCl)c1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 199.59
CAS: 99-47-8

Physical Properties

Property code	Value	Unit	Source
gf	13.96	kJ/mol	Joback Method
hf	-122.47	kJ/mol	Joback Method
hfus	27.29	kJ/mol	Joback Method
hvap	64.06	kJ/mol	Joback Method
log10ws	-2.94		Crippen Method
logp	2.016		Crippen Method
mcvol	131.050	ml/mol	McGowan Method
pc	3754.57	kPa	Joback Method
tb	657.24	K	Joback Method
tc	911.94	K	Joback Method
tf	442.32	K	Joback Method
vc	0.512	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	296.96	J/mol×K	657.24	Joback Method
cpg	306.70	J/mol×K	699.69	Joback Method
cpg	315.58	J/mol×K	742.14	Joback Method
cpg	323.66	J/mol×K	784.59	Joback Method
cpg	330.99	J/mol×K	827.04	Joback Method
cpg	337.61	J/mol×K	869.49	Joback Method
cpg	343.56	J/mol×K	911.94	Joback Method
hsubt	109.10	kJ/mol	321.00	NIST Webbook

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=C99478&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
hsubt:	Enthalpy of sublimation at a given temperature
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