4-Methyl-3-nitrobenzoyl chloride

Other names: 3-Nitro-p-toluyl chloride
Benzoyl chloride, 4-methyl-3-nitro-
Inchi: InChI=1S/C8H6ClNO3/c1-5-2-3-6(8(9)11)4-7(5)10(12)13/h2-4H,1H3
InchiKey: DXMHBBURYDVYAI-UHFFFAOYSA-N
Formula: C8H6ClNO3
SMILES: Cc1ccc(C(=O)Cl)cc1[N+](=O)[O-]
Mol. weight [g/mol]: 199.59
CAS: 10397-30-5

Physical Properties

Property code	Value	Unit	Source
gf	4.33	kJ/mol	Joback Method
hf	-133.94	kJ/mol	Joback Method
hfus	26.90	kJ/mol	Joback Method
hvap	64.72	kJ/mol	Joback Method
log10ws	-3.49		Crippen Method
logp	2.282		Crippen Method
mcvol	131.050	ml/mol	McGowan Method
pc	3686.49	kPa	Joback Method
tb	662.22	K	Joback Method
tc	917.82	K	Joback Method
tf	454.84	K	Joback Method
vc	0.512	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	295.22	J/mol×K	662.22	Joback Method
cpg	304.78	J/mol×K	704.82	Joback Method
cpg	313.53	J/mol×K	747.42	Joback Method
cpg	321.52	J/mol×K	790.02	Joback Method
cpg	328.78	J/mol×K	832.62	Joback Method
cpg	335.35	J/mol×K	875.22	Joback Method
cpg	341.26	J/mol×K	917.82	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	434.00 ± 1.00	K	2.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10397305&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume