2-Chloro-5-nitrobenzoyl chloride

Other names: Benzoyl chloride, 2-chloro-5-nitro-
Inchi: InChI=1S/C7H3Cl2NO3/c8-6-2-1-4(10(12)13)3-5(6)7(9)11/h1-3H
InchiKey: OGLKKYALUKXVPQ-UHFFFAOYSA-N
Formula: C7H3Cl2NO3
SMILES: O=C(Cl)c1cc([N+](=O)[O-])ccc1Cl
Mol. weight [g/mol]: 220.01
CAS: 25784-91-2

Physical Properties

Property code	Value	Unit	Source
gf	-16.02	kJ/mol	Joback Method
hf	-129.04	kJ/mol	Joback Method
hfus	28.50	kJ/mol	Joback Method
hvap	66.88	kJ/mol	Joback Method
log10ws	-3.70		Crippen Method
logp	2.627		Crippen Method
mcvol	129.200	ml/mol	McGowan Method
pc	3965.51	kPa	Joback Method
tb	676.77	K	Joback Method
tc	940.91	K	Joback Method
tf	473.49	K	Joback Method
vc	0.505	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	267.35	J/mol×K	676.77	Joback Method
cpg	274.94	J/mol×K	720.79	Joback Method
cpg	281.80	J/mol×K	764.82	Joback Method
cpg	287.96	J/mol×K	808.84	Joback Method
cpg	293.47	J/mol×K	852.86	Joback Method
cpg	298.37	J/mol×K	896.88	Joback Method
cpg	302.69	J/mol×K	940.91	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C25784912&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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