Benzoyl chloride, 3,5-dinitro-

Other names:	3,5-Dinitrobenzoic acid chloride
	3,5-Dinitrobenzoyl chloride
Inchi:	InChI=1S/C7H3ClN2O5/c8-7(11)4-1-5(9(12)13)3-6(2-4)10(14)15/h1-3H
InchiKey:	NNOHXABAQAGKRZ-UHFFFAOYSA-N
Formula:	C7H3ClN2O5
SMILES:	O=C(Cl)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
Mol. weight [g/mol]:	230.56
CAS:	99-33-2

Physical Properties

Property code	Value	Unit	Source
gf	31.46	kJ/mol	Joback Method
hf	-124.06	kJ/mol	Joback Method
hfus	35.67	kJ/mol	Joback Method
hvap	79.09	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	1.882		Crippen Method
mcvol	134.380	ml/mol	McGowan Method
pc	4222.04	kPa	Joback Method
rinpol	1706.00		NIST Webbook
tb	791.18	K	Joback Method
tc	1070.74	K	Joback Method
tf	587.18	K	Joback Method
vc	0.538	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	320.45	J/mol×K	791.18	Joback Method
cpg	327.44	J/mol×K	837.77	Joback Method
cpg	333.60	J/mol×K	884.37	Joback Method
cpg	338.98	J/mol×K	930.96	Joback Method
cpg	343.62	J/mol×K	977.55	Joback Method
cpg	347.58	J/mol×K	1024.15	Joback Method

cpg	350.92	J/mol×K	1070.74	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	469.20	K	1.50	NIST Webbook

Sources

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=C99332&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume