

5-Isobenzofurancarbonyl chloride, 1,3-dihydro-1,3-dioxo-

Other names:	Phthalic anhydride, 4-(chloroformyl)- Anhydrotrimellitic acid chloride Trimellitic acid anhydride chloride Trimellitic acid anhydride 4-monoacid chloride Trimellitic anhydride acid chloride Trimellitic anhydride chloride Trimellitic anhydride monoacid chloride Trimellitic anhydride monochloride 1,3-Benzofurandione-5-carbonyl chloride 4-(Chlorocarbonyl)phthalic anhydride 4-(Chloroformyl)phthalic anhydride 4-(Chlorocarboxy)benzenedicarboxylic anhydride Phthalic , 4-(chloroformyl)-,anhydride NSC 89728
Inchi:	InChI=1S/C9H3ClO4/c10-7(11)4-1-2-5-6(3-4)9(13)14-8(5)12/h1-3H
InchiKey:	NJMOHBDCGXJLNJ-UHFFFAOYSA-N
Formula:	C9H3ClO4
SMILES:	O=C(Cl)c1ccc2c(c1)C(=O)OC2=O
Mol. weight [g/mol]:	210.57
CAS:	1204-28-0

Physical Properties

Property code	Value	Unit	Source
gf	-285.64	kJ/mol	Joback Method
hf	-458.08	kJ/mol	Joback Method
hfus	22.19	kJ/mol	Joback Method
hvap	63.58	kJ/mol	Joback Method
log10ws	-2.82		Crippen Method
logp	1.376		Crippen Method
mcvol	125.870	ml/mol	McGowan Method
pc	4266.28	kPa	Joback Method
tb	707.26	K	Joback Method
tc	973.03	K	Joback Method
tf	507.69	K	Joback Method
vc	0.479	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.57	J/mol×K	707.26	Joback Method
cpg	309.26	J/mol×K	751.55	Joback Method
cpg	318.09	J/mol×K	795.85	Joback Method
cpg	326.05	J/mol×K	840.14	Joback Method
cpg	333.11	J/mol×K	884.44	Joback Method
cpg	339.26	J/mol×K	928.73	Joback Method
cpg	344.48	J/mol×K	973.03	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1204280&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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