

Benzoic acid, 2-chloro-, phenyl ester

Other names:	2-Chlorobenzoic acid, phenyl ester Phenyl 2-chlorobenzoate
Inchi:	InChI=1S/C13H9ClO2/c14-12-9-5-4-8-11(12)13(15)16-10-6-2-1-3-7-10/h1-9H
InchiKey:	RBKABBZAJGDBFA-UHFFFAOYSA-N
Formula:	C13H9ClO2
SMILES:	O=C(Oc1ccccc1)c1ccccc1Cl
Mol. weight [g/mol]:	232.66
CAS:	41998-16-7

Physical Properties

Property code	Value	Unit	Source
gf	27.92	kJ/mol	Joback Method
hf	-110.60	kJ/mol	Joback Method
hfus	24.10	kJ/mol	Joback Method
hvap	63.29	kJ/mol	Joback Method
log10ws	-4.24		Crippen Method
logp	3.559		Crippen Method
mvol	166.190	ml/mol	McGowan Method
pc	3052.41	kPa	Joback Method
tb	668.90	K	Joback Method
tc	920.71	K	Joback Method
tf	403.71	K	Joback Method
vc	0.621	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	389.69	J/molxK	668.90	Joback Method
cpg	402.92	J/molxK	710.87	Joback Method
cpg	415.01	J/molxK	752.84	Joback Method
cpg	426.00	J/molxK	794.80	Joback Method
cpg	435.96	J/molxK	836.77	Joback Method
cpg	444.92	J/molxK	878.74	Joback Method
cpg	452.94	J/molxK	920.71	Joback Method

dvisc	0.0012209	Paxs	403.71	Joback Method
dvisc	0.0007326	Paxs	447.91	Joback Method
dvisc	0.0004818	Paxs	492.11	Joback Method
dvisc	0.0003395	Paxs	536.31	Joback Method
dvisc	0.0002524	Paxs	580.50	Joback Method
dvisc	0.0001956	Paxs	624.70	Joback Method
dvisc	0.0001568	Paxs	668.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C41998167&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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
dvisc:	Dynamic viscosity
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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