

2-Chlorobenzoic acid, 2-phenylethyl ester

Other names:	Benzoic acid, 2-chloro, 2-phenylethyl ester 2-Phenylethyl 2-chlorobenzoate
Inchi:	InChI=1S/C15H13ClO2/c16-14-9-5-4-8-13(14)15(17)18-11-10-12-6-2-1-3-7-12/h1-9H,10
InchiKey:	FANZVPUMGJHASY-UHFFFAOYSA-N
Formula:	C15H13ClO2
SMILES:	O=C(OCCc1ccccc1)c1ccccc1Cl
Mol. weight [g/mol]:	260.72
CAS:	104856-44-2

Physical Properties

Property code	Value	Unit	Source
gf	44.76	kJ/mol	Joback Method
hf	-151.88	kJ/mol	Joback Method
hfus	29.28	kJ/mol	Joback Method
hvap	67.74	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	3.739		Crippen Method
mvol	194.370	ml/mol	McGowan Method
pc	2495.01	kPa	Joback Method
rinpol	1989.00		NIST Webbook
rinpol	2006.00		NIST Webbook
rinpol	2020.00		NIST Webbook
rinpol	2037.00		NIST Webbook
rinpol	1989.00		NIST Webbook
rinpol	1987.00		NIST Webbook
rinpol	2001.00		NIST Webbook
rinpol	1953.00		NIST Webbook
rinpol	1953.00		NIST Webbook
rinpol	2037.00		NIST Webbook
rinpol	1969.00		NIST Webbook
rinpol	1987.00		NIST Webbook
ripol	2927.00		NIST Webbook
ripol	2959.00		NIST Webbook
ripol	2994.00		NIST Webbook
ripol	2927.00		NIST Webbook
ripol	2979.00		NIST Webbook
ripol	2968.00		NIST Webbook

tb	714.66	K	Joback Method
tc	955.69	K	Joback Method
tf	426.25	K	Joback Method
vc	0.733	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	491.15	J/mol×K	714.66	Joback Method
cpg	551.20	J/mol×K	915.52	Joback Method
cpg	541.33	J/mol×K	875.35	Joback Method
cpg	530.44	J/mol×K	835.17	Joback Method
cpg	518.48	J/mol×K	795.00	Joback Method
cpg	505.40	J/mol×K	754.83	Joback Method
cpg	560.11	J/mol×K	955.69	Joback Method
dvisc	0.0001258	Paxs	714.66	Joback Method
dvisc	0.0001583	Paxs	666.59	Joback Method
dvisc	0.0002064	Paxs	618.52	Joback Method
dvisc	0.0002815	Paxs	570.45	Joback Method
dvisc	0.0004066	Paxs	522.39	Joback Method
dvisc	0.0006325	Paxs	474.32	Joback Method
dvisc	0.0010871	Paxs	426.25	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C104856442&Units=SI

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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