

1-Phenylethyl 2-chlorobenzoate

Inchi:	InChI=1S/C15H13ClO2/c1-11(12-7-3-2-4-8-12)18-15(17)13-9-5-6-10-14(13)16/h2-11H,1
InchiKey:	UKIZIOCBMHEFMW-UHFFFAOYSA-N
Formula:	C15H13ClO2
SMILES:	CC(OC(=O)c1ccccc1Cl)c1ccccc1
Mol. weight [g/mol]:	260.72

Physical Properties

Property code	Value	Unit	Source
gf	42.32	kJ/mol	Joback Method
hf	-157.16	kJ/mol	Joback Method
hfus	25.76	kJ/mol	Joback Method
hvap	67.35	kJ/mol	Joback Method
log10ws	-4.89		Crippen Method
logp	4.258		Crippen Method
mcvol	194.370	ml/mol	McGowan Method
pc	2515.07	kPa	Joback Method
rinpol	1905.00		NIST Webbook
rinpol	1949.00		NIST Webbook
rinpol	1882.00		NIST Webbook
rinpol	1897.00		NIST Webbook
rinpol	1912.00		NIST Webbook
rinpol	1924.00		NIST Webbook
rinpol	1937.00		NIST Webbook
rinpol	1882.00		NIST Webbook
rinpol	1905.00		NIST Webbook
rinpol	1917.00		NIST Webbook
rinpol	1949.00		NIST Webbook
ripol	2839.00		NIST Webbook
ripol	2807.00		NIST Webbook
ripol	2802.00		NIST Webbook
ripol	2760.00		NIST Webbook
ripol	2786.00		NIST Webbook
ripol	2814.00		NIST Webbook
ripol	2760.00		NIST Webbook
ripol	2807.00		NIST Webbook
tb	714.22	K	Joback Method
tc	960.09	K	Joback Method

tf	411.25	K	Joback Method
vc	0.727	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	491.72	J/molxK	714.22	Joback Method
cpg	552.70	J/molxK	919.12	Joback Method
cpg	542.75	J/molxK	878.14	Joback Method
cpg	531.74	J/molxK	837.16	Joback Method
cpg	519.60	J/molxK	796.18	Joback Method
cpg	506.28	J/molxK	755.20	Joback Method
cpg	561.64	J/molxK	960.09	Joback Method
dvisc	0.0001162	Paxs	714.22	Joback Method
dvisc	0.0001487	Paxs	663.73	Joback Method
dvisc	0.0001982	Paxs	613.23	Joback Method
dvisc	0.0002782	Paxs	562.74	Joback Method
dvisc	0.0004174	Paxs	512.24	Joback Method
dvisc	0.0006843	Paxs	461.75	Joback Method
dvisc	0.0012667	Paxs	411.25	Joback Method

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=R34977&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
m_{cvol}:	McGowan's characteristic volume
p_c:	Critical Pressure
r_{inpol}:	Non-polar retention indices
r_{ipol}:	Polar retention indices
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature
t_f:	Normal melting (fusion) point
v_c:	Critical Volume

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