2-Phenylethyl 3-chlorobenzoate

Other names: Benzoic acid, 3-chloro, 2-phenylethyl ester
Inchi: InChI=1S/C15H13ClO2/c16-14-8-4-7-13(11-14)15(17)18-10-9-12-5-2-1-3-6-12/h1-8,11H,
InchiKey: HVYMOPGTMRUTRG-UHFFFAOYSA-N
Formula: C15H13ClO2
SMILES: O=C(OCCc1ccccc1)c1cccc(Cl)c1
Mol. weight [g/mol]: 260.72

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
mcvol	194.370	ml/mol	McGowan Method
pc	2495.01	kPa	Joback Method
rinpol	1945.00		NIST Webbook
rinpol	2024.00		NIST Webbook
rinpol	1978.00		NIST Webbook
rinpol	1977.00		NIST Webbook
rinpol	1990.00		NIST Webbook
rinpol	1945.00		NIST Webbook
rinpol	2024.00		NIST Webbook
rinpol	1977.00		NIST Webbook
rinpol	1962.00		NIST Webbook
rinpol	1993.00		NIST Webbook
rinpol	2007.00		NIST Webbook
rinpol	1978.00		NIST Webbook
ripol	2841.00		NIST Webbook
ripol	2873.00		NIST Webbook
ripol	2841.00		NIST Webbook
ripol	2888.00		NIST Webbook
ripol	2869.00		NIST Webbook
ripol	2888.00		NIST Webbook
ripol	2841.00		NIST Webbook
ripol	2905.00		NIST Webbook

tb	714.66	K	Joback Method
tc	955.69	K	Joback Method
tf	426.25	K	Joback Method
vc	0.733	m3/kmol	Joback Method

Temperature Dependent Properties

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

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R34909&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