1-Phenylethyl 3-chlorobenzoate

Inchi: InChI=1S/C15H13ClO2/c1-11(12-6-3-2-4-7-12)18-15(17)13-8-5-9-14(16)10-13/h2-11H,1
InchiKey: TZHYMJYOHPXXRU-UHFFFAOYSA-N
Formula: C15H13ClO2
SMILES: CC(OC(=O)c1cccc(Cl)c1)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	1949.00		NIST Webbook
rinpol	1936.00		NIST Webbook
rinpol	1923.00		NIST Webbook
rinpol	1894.00		NIST Webbook
rinpol	1904.00		NIST Webbook
rinpol	1915.00		NIST Webbook
rinpol	1910.00		NIST Webbook
rinpol	1880.00		NIST Webbook
ripol	2692.00		NIST Webbook
ripol	2745.00		NIST Webbook
ripol	2771.00		NIST Webbook
ripol	2739.00		NIST Webbook
ripol	2722.00		NIST Webbook
ripol	2692.00		NIST Webbook
ripol	2739.00		NIST Webbook
ripol	2717.00		NIST Webbook
tb	714.22	K	Joback Method
tc	960.09	K	Joback Method
tf	411.25	K	Joback Method
vc	0.727	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	491.72	J/mol×K	714.22	Joback Method
cpg	506.28	J/mol×K	755.20	Joback Method
cpg	519.60	J/mol×K	796.18	Joback Method
cpg	531.74	J/mol×K	837.16	Joback Method
cpg	542.75	J/mol×K	878.14	Joback Method
cpg	552.70	J/mol×K	919.12	Joback Method
cpg	561.64	J/mol×K	960.09	Joback Method
dvisc	0.0012667	Pa×s	411.25	Joback Method
dvisc	0.0006843	Pa×s	461.75	Joback Method
dvisc	0.0004174	Pa×s	512.24	Joback Method
dvisc	0.0002782	Pa×s	562.74	Joback Method
dvisc	0.0001982	Pa×s	613.23	Joback Method
dvisc	0.0001487	Pa×s	663.73	Joback Method
dvisc	0.0001162	Pa×s	714.22	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=R34981&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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