Butyric acid, 2-phenyl-, 3-chlorophenyl ester

Inchi: InChI=1S/C16H15ClO2/c1-2-15(12-7-4-3-5-8-12)16(18)19-14-10-6-9-13(17)11-14/h3-11,
InchiKey: OHIKIFPKDVGHPY-UHFFFAOYSA-N
Formula: C16H15ClO2
SMILES: CCC(C(=O)Oc1cccc(Cl)c1)c1ccccc1
Mol. weight [g/mol]: 274.74

Physical Properties

Property code	Value	Unit	Source
gf	50.74	kJ/mol	Joback Method
hf	-177.80	kJ/mol	Joback Method
hfus	28.35	kJ/mol	Joback Method
hvap	69.58	kJ/mol	Joback Method
log10ws	-4.89		Crippen Method
logp	4.439		Crippen Method
mcvol	208.460	ml/mol	McGowan Method
pc	2289.32	kPa	Joback Method
rinpol	1998.00		NIST Webbook
rinpol	1998.00		NIST Webbook
tb	737.10	K	Joback Method
tc	977.90	K	Joback Method
tf	422.52	K	Joback Method
vc	0.782	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	544.33	J/mol×K	737.10	Joback Method
cpg	607.05	J/mol×K	937.77	Joback Method
cpg	596.76	J/mol×K	897.64	Joback Method
cpg	585.40	J/mol×K	857.50	Joback Method
cpg	572.91	J/mol×K	817.37	Joback Method
cpg	559.24	J/mol×K	777.23	Joback Method
cpg	616.32	J/mol×K	977.90	Joback Method
dvisc	0.0001031	Pa×s	737.10	Joback Method

dvisc	0.0001325	Pa×s	684.67	Joback Method
dvisc	0.0001774	Pa×s	632.24	Joback Method
dvisc	0.0002504	Pa×s	579.81	Joback Method
dvisc	0.0003785	Pa×s	527.38	Joback Method
dvisc	0.0006268	Pa×s	474.95	Joback Method
dvisc	0.0011764	Pa×s	422.52	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=U406863&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume