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

Inchi: InChI=1S/C16H14Cl2O2/c1-2-12(11-7-4-3-5-8-11)16(19)20-14-10-6-9-13(17)15(14)18/h3

InchiKey: HTFWNXCXBGHKCV-UHFFFAOYSA-N

Formula: C16H14Cl2O2

SMILES: CCC(C(=O)Oc1cccc(Cl)c1Cl)c1ccccc1

Mol. weight [g/mol]: 309.19

Physical Properties

Property code	Value	Unit	Source
gf	29.18	kJ/mol	Joback Method
hf	-205.01	kJ/mol	Joback Method
hfus	32.16	kJ/mol	Joback Method
hvap	74.62	kJ/mol	Joback Method
log10ws	-5.57		Crippen Method
logp	5.093		Crippen Method
mcvol	220.700	ml/mol	McGowan Method
pc	2179.52	kPa	Joback Method
rinpol	2199.00		NIST Webbook
rinpol	2199.00		NIST Webbook
tb	779.51	K	Joback Method
tc	1023.23	K	Joback Method
tf	464.96	K	Joback Method
vc	0.832	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	566.97	J/mol×K	779.51	Joback Method
cpg	622.70	J/mol×K	982.61	Joback Method
cpg	613.71	J/mol×K	941.99	Joback Method
cpg	603.70	J/mol×K	901.37	Joback Method
cpg	592.60	J/mol×K	860.75	Joback Method
cpg	580.38	J/mol×K	820.13	Joback Method
cpg	630.72	J/mol×K	1023.23	Joback Method
dvisc	0.0000928	Pa×s	779.51	Joback Method

dvisc	0.0001172	Pa×s	727.09	Joback Method
dvisc	0.0001536	Pa×s	674.66	Joback Method
dvisc	0.0002107	Pa×s	622.24	Joback Method
dvisc	0.0003063	Pa×s	569.81	Joback Method
dvisc	0.0004804	Pa×s	517.38	Joback Method
dvisc	0.0008337	Pa×s	464.96	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=U406865&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume