Butyric acid, 2-phenyl-, 2,2-dichloroethyl ester

Inchi: InChI=1S/C12H14Cl2O2/c1-2-10(9-6-4-3-5-7-9)12(15)16-8-11(13)14/h3-7,10-11H,2,8H2
InchiKey: HSMIMZKVUUSGOL-UHFFFAOYSA-N
Formula: C12H14Cl2O2
SMILES: CCC(C(=O)OCC(Cl)Cl)c1ccccc1
Mol. weight [g/mol]: 261.14

Physical Properties

Property code	Value	Unit	Source
gf	-100.09	kJ/mol	Joback Method
hf	-341.32	kJ/mol	Joback Method
hfus	25.01	kJ/mol	Joback Method
hvap	61.73	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	3.527		Crippen Method
mcvol	188.100	ml/mol	McGowan Method
pc	2377.22	kPa	Joback Method
rinpol	1672.00		NIST Webbook
rinpol	1672.00		NIST Webbook
tb	650.91	K	Joback Method
tc	872.91	K	Joback Method
tf	353.42	K	Joback Method
vc	0.710	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	449.33	J/mol×K	650.91	Joback Method
cpg	509.26	J/mol×K	835.91	Joback Method
cpg	499.06	J/mol×K	798.91	Joback Method
cpg	488.00	J/mol×K	761.91	Joback Method
cpg	476.05	J/mol×K	724.91	Joback Method
cpg	463.17	J/mol×K	687.91	Joback Method
cpg	518.64	J/mol×K	872.91	Joback Method
dvisc	0.0001406	Pa×s	650.91	Joback Method

dvisc	0.0001873	Pa×s	601.33	Joback Method
dvisc	0.0002625	Pa×s	551.75	Joback Method
dvisc	0.0003934	Pa×s	502.16	Joback Method
dvisc	0.0006441	Pa×s	452.58	Joback Method
dvisc	0.0011908	Pa×s	403.00	Joback Method
dvisc	0.0026155	Pa×s	353.42	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=U406857&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