Butyric acid, 2-phenyl-, 2-chloro-6-fluorophenyl ester

Inchi: InChI=1S/C16H14ClFO2/c1-2-12(11-7-4-3-5-8-11)16(19)20-15-13(17)9-6-10-14(15)18/h3

InchiKey: LGRJZYNTXIEPJJ-UHFFFAOYSA-N

Formula: C16H14ClFO2

SMILES: CCC(C(=O)Oc1c(F)cccc1Cl)c1ccccc1

Mol. weight [g/mol]: 292.73

Physical Properties

Property code	Value	Unit	Source
gf	-153.70	kJ/mol	Joback Method
hf	-385.38	kJ/mol	Joback Method
hfus	31.04	kJ/mol	Joback Method
hvap	69.42	kJ/mol	Joback Method
log10ws	-5.22		Crippen Method
logp	4.578		Crippen Method
mcvol	210.230	ml/mol	McGowan Method
pc	2163.33	kPa	Joback Method
rinpol	1966.00		NIST Webbook
rinpol	1966.00		NIST Webbook
tb	741.35	K	Joback Method
tc	972.78	K	Joback Method
tf	435.63	K	Joback Method
vc	0.800	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	550.96	J/mol×K	741.35	Joback Method
cpg	565.03	J/mol×K	779.92	Joback Method
cpg	577.97	J/mol×K	818.49	Joback Method
cpg	589.83	J/mol×K	857.06	Joback Method
cpg	600.64	J/mol×K	895.63	Joback Method
cpg	610.46	J/mol×K	934.21	Joback Method
cpg	619.34	J/mol×K	972.78	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406862&Units=SI
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

Legend

cpg:	Ideal gas heat capacity
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