3-Phenylpropionic acid, 2-bromo-4-fluorophenyl ester

Inchi: InChI=1S/C15H12BrFO2/c16-13-10-12(17)7-8-14(13)19-15(18)9-6-11-4-2-1-3-5-11/h1-5,

InchiKey: SVZVYAAOCLXEJA-UHFFFAOYSA-N

Formula: C15H12BrFO2

SMILES: O=C(CCc1ccccc1)Oc1ccc(F)cc1Br

Mol. weight [g/mol]: 323.16

Physical Properties

Property code	Value	Unit	Source
gf	-133.43	kJ/mol	Joback Method
hf	-317.39	kJ/mol	Joback Method
hfus	33.06	kJ/mol	Joback Method
hvap	69.63	kJ/mol	Joback Method
log10ws	-5.31		Crippen Method
logp	4.126		Crippen Method
mcvol	201.400	ml/mol	McGowan Method
pc	2613.74	kPa	Joback Method
rinpol	2008.00		NIST Webbook
rinpol	2008.00		NIST Webbook
tb	747.64	K	Joback Method
tc	986.46	K	Joback Method
tf	469.24	K	Joback Method
vc	0.763	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	508.66	J/mol×K	747.64	Joback Method
cpg	521.57	J/mol×K	787.44	Joback Method
cpg	533.41	J/mol×K	827.25	Joback Method
cpg	544.23	J/mol×K	867.05	Joback Method
cpg	554.09	J/mol×K	906.85	Joback Method
cpg	563.05	J/mol×K	946.66	Joback Method
cpg	571.15	J/mol×K	986.46	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299023&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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