Diglycolic acid, 2-bromo-4-fluorophenyl butyl ester

Inchi: InChI=1S/C14H16BrFO5/c1-2-3-6-20-13(17)8-19-9-14(18)21-12-5-4-10(16)7-11(12)15/h4

InchiKey: YFOVWLCIKIQRFM-UHFFFAOYSA-N

Formula: C14H16BrFO5

SMILES: CCCCOC(=O)COCC(=O)Oc1ccc(F)cc1Br

Mol. weight [g/mol]: 363.18

Physical Properties

Property code	Value	Unit	Source
gf	-593.18	kJ/mol	Joback Method
hf	-910.30	kJ/mol	Joback Method
hfus	40.41	kJ/mol	Joback Method
hvap	76.70	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	2.853		Crippen Method
mcvol	224.380	ml/mol	McGowan Method
pc	2139.38	kPa	Joback Method
rinpol	2793.00		NIST Webbook
rinpol	2793.00		NIST Webbook
tb	796.79	K	Joback Method
tc	1005.29	K	Joback Method
tf	525.94	K	Joback Method
vc	0.858	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	610.01	J/mol×K	796.79	Joback Method
cpg	621.94	J/mol×K	831.54	Joback Method
cpg	632.95	J/mol×K	866.29	Joback Method
cpg	643.04	J/mol×K	901.04	Joback Method
cpg	652.20	J/mol×K	935.79	Joback Method
cpg	660.43	J/mol×K	970.54	Joback Method
cpg	667.73	J/mol×K	1005.29	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381994&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