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

Inchi: InChI=1S/C14H16BrFO5/c1-9(2)6-20-13(17)7-19-8-14(18)21-12-4-3-10(16)5-11(12)15/h3

InchiKey: OKVXSKIOEAFEHK-UHFFFAOYSA-N

Formula: C14H16BrFO5

SMILES: CC(C)COC(=O)COCC(=O)Oc1ccc(F)cc1Br

Mol. weight [g/mol]: 363.18

Physical Properties

Property code	Value	Unit	Source
gf	-595.62	kJ/mol	Joback Method
hf	-915.58	kJ/mol	Joback Method
hfus	36.88	kJ/mol	Joback Method
hvap	76.31	kJ/mol	Joback Method
log10ws	-3.50		Crippen Method
logp	2.709		Crippen Method
mcvol	224.380	ml/mol	McGowan Method
pc	2155.30	kPa	Joback Method
rinpol	2727.00		NIST Webbook
rinpol	2727.00		NIST Webbook
tb	796.35	K	Joback Method
tc	1007.69	K	Joback Method
tf	510.94	K	Joback Method
vc	0.852	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	610.60	J/mol×K	796.35	Joback Method
cpg	622.69	J/mol×K	831.57	Joback Method
cpg	633.82	J/mol×K	866.80	Joback Method
cpg	644.00	J/mol×K	902.02	Joback Method
cpg	653.21	J/mol×K	937.25	Joback Method
cpg	661.45	J/mol×K	972.47	Joback Method
cpg	668.72	J/mol×K	1007.69	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=U381993&Units=SI

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