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

Inchi: InChI=1S/C13H14BrFO5/c1-2-5-19-12(16)7-18-8-13(17)20-11-4-3-9(15)6-10(11)14/h3-4,

InchiKey: WMHFTEYKVPTGBP-UHFFFAOYSA-N

Formula: C13H14BrFO5

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

Mol. weight [g/mol]: 349.15

Physical Properties

Property code	Value	Unit	Source
gf	-601.60	kJ/mol	Joback Method
hf	-889.66	kJ/mol	Joback Method
hfus	37.82	kJ/mol	Joback Method
hvap	74.47	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	2.463		Crippen Method
mcvol	210.290	ml/mol	McGowan Method
pc	2342.82	kPa	Joback Method
rinpol	2652.00		NIST Webbook
rinpol	2652.00		NIST Webbook
tb	773.91	K	Joback Method
tc	984.17	K	Joback Method
tf	514.67	K	Joback Method
vc	0.801	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	556.10	J/mol×K	773.91	Joback Method
cpg	567.65	J/mol×K	808.95	Joback Method
cpg	578.32	J/mol×K	844.00	Joback Method
cpg	588.11	J/mol×K	879.04	Joback Method
cpg	597.02	J/mol×K	914.09	Joback Method
cpg	605.04	J/mol×K	949.13	Joback Method
cpg	612.16	J/mol×K	984.17	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381992&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