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

Inchi: InChI=1S/C12H12BrFO5/c1-2-18-11(15)6-17-7-12(16)19-10-4-3-8(14)5-9(10)13/h3-5H,2

InchiKey: AAURJXDVRUDXIE-UHFFFAOYSA-N

Formula: C12H12BrFO5

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

Mol. weight [g/mol]: 335.12

Physical Properties

Property code	Value	Unit	Source
gf	-610.02	kJ/mol	Joback Method
hf	-869.02	kJ/mol	Joback Method
hfus	35.23	kJ/mol	Joback Method
hvap	72.25	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.073		Crippen Method
mcvol	196.200	ml/mol	McGowan Method
pc	2576.72	kPa	Joback Method
rinpol	2518.00		NIST Webbook
tb	751.03	K	Joback Method
tc	963.60	K	Joback Method
tf	503.40	K	Joback Method
vc	0.746	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.30	J/mol×K	751.03	Joback Method
cpg	514.39	J/mol×K	786.46	Joback Method
cpg	524.66	J/mol×K	821.89	Joback Method
cpg	534.09	J/mol×K	857.31	Joback Method
cpg	542.69	J/mol×K	892.74	Joback Method
cpg	550.43	J/mol×K	928.17	Joback Method
cpg	557.32	J/mol×K	963.60	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381991&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