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

Inchi: InChI=1S/C18H24BrFO5/c1-2-3-4-5-6-7-10-24-17(21)12-23-13-18(22)25-16-9-8-14(20)11

InchiKey: JLAFOGBGDRKAOM-UHFFFAOYSA-N

Formula: C18H24BrFO5

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

Mol. weight [g/mol]: 419.28

Physical Properties

Property code	Value	Unit	Source
gf	-559.50	kJ/mol	Joback Method
hf	-992.86	kJ/mol	Joback Method
hfus	50.77	kJ/mol	Joback Method
hvap	85.60	kJ/mol	Joback Method
log10ws	-5.42		Crippen Method
logp	4.414		Crippen Method
mcvol	280.740	ml/mol	McGowan Method
pc	1542.71	kPa	Joback Method
rinpol	3321.00		NIST Webbook
rinpol	3321.00		NIST Webbook
tb	888.31	K	Joback Method
tc	1096.13	K	Joback Method
tf	571.02	K	Joback Method
vc	1.081	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	835.03	J/mol×K	888.31	Joback Method
cpg	848.07	J/mol×K	922.95	Joback Method
cpg	859.98	J/mol×K	957.58	Joback Method
cpg	870.77	J/mol×K	992.22	Joback Method
cpg	880.45	J/mol×K	1026.86	Joback Method
cpg	889.02	J/mol×K	1061.49	Joback Method
cpg	896.51	J/mol×K	1096.13	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381999&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