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

Inchi: InChI=1S/C15H18BrFO5/c1-2-3-4-7-21-14(18)9-20-10-15(19)22-13-6-5-11(17)8-12(13)1

InchiKey: PMNQKJUELUVKFP-UHFFFAOYSA-N

Formula: C15H18BrFO5

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

Mol. weight [g/mol]: 377.20

Physical Properties

Property code	Value	Unit	Source
gf	-584.76	kJ/mol	Joback Method
hf	-930.94	kJ/mol	Joback Method
hfus	43.00	kJ/mol	Joback Method
hvap	78.92	kJ/mol	Joback Method
log10ws	-4.16		Crippen Method
logp	3.244		Crippen Method
mcvol	238.470	ml/mol	McGowan Method
pc	1961.34	kPa	Joback Method
rinpol	2936.00		NIST Webbook
tb	819.67	K	Joback Method
tc	1027.00	K	Joback Method
tf	537.21	K	Joback Method
vc	0.913	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	664.93	J/mol×K	819.67	Joback Method
cpg	677.20	J/mol×K	854.23	Joback Method
cpg	688.49	J/mol×K	888.78	Joback Method
cpg	698.82	J/mol×K	923.34	Joback Method
cpg	708.18	J/mol×K	957.89	Joback Method
cpg	716.56	J/mol×K	992.45	Joback Method
cpg	723.98	J/mol×K	1027.00	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381995&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