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

Inchi: InChI=1S/C17H22BrFO5/c1-2-3-4-5-6-9-23-16(20)11-22-12-17(21)24-15-8-7-13(19)10-14

InchiKey: KIRPFSPZTADQAC-UHFFFAOYSA-N

Formula: C17H22BrFO5

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

Mol. weight [g/mol]: 405.26

Physical Properties

Property code	Value	Unit	Source
gf	-567.92	kJ/mol	Joback Method
hf	-972.22	kJ/mol	Joback Method
hfus	48.18	kJ/mol	Joback Method
hvap	83.38	kJ/mol	Joback Method
log10ws	-5.00		Crippen Method
logp	4.024		Crippen Method
mcvol	266.650	ml/mol	McGowan Method
pc	1665.97	kPa	Joback Method
rinpol	3203.00		NIST Webbook
rinpol	3203.00		NIST Webbook
tb	865.43	K	Joback Method
tc	1072.37	K	Joback Method
tf	559.75	K	Joback Method
vc	1.026	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	777.52	J/mol×K	865.43	Joback Method
cpg	790.33	J/mol×K	899.92	Joback Method
cpg	802.06	J/mol×K	934.41	Joback Method
cpg	812.74	J/mol×K	968.90	Joback Method
cpg	822.35	J/mol×K	1003.39	Joback Method
cpg	830.90	J/mol×K	1037.88	Joback Method
cpg	838.41	J/mol×K	1072.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381998&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