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

Inchi: InChI=1S/C16H20BrFO5/c1-11(2)4-3-7-22-15(19)9-21-10-16(20)23-14-6-5-12(18)8-13(1
InchiKey: VHUQZNHADJVWID-UHFFFAOYSA-N
Formula: C16H20BrFO5
SMILES: CC(C)CCCOC(=O)COCC(=O)Oc1ccc(F)cc1Br
Mol. weight [g/mol]: 391.23

Physical Properties

Property code	Value	Unit	Source
gf	-578.78	kJ/mol	Joback Method
hf	-956.86	kJ/mol	Joback Method
hfus	42.06	kJ/mol	Joback Method
hvap	80.76	kJ/mol	Joback Method
log10ws	-4.34		Crippen Method
logp	3.490		Crippen Method
mcvol	252.560	ml/mol	McGowan Method
pc	1816.95	kPa	Joback Method
rinpol	3022.00		NIST Webbook
rinpol	3022.00		NIST Webbook
tb	842.11	K	Joback Method
tc	1051.12	K	Joback Method
tf	533.48	K	Joback Method
vc	0.964	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	721.36	J/mol×K	842.11	Joback Method
cpg	734.03	J/mol×K	876.94	Joback Method
cpg	745.65	J/mol×K	911.78	Joback Method
cpg	756.23	J/mol×K	946.61	Joback Method
cpg	765.75	J/mol×K	981.45	Joback Method
cpg	774.23	J/mol×K	1016.28	Joback Method
cpg	781.67	J/mol×K	1051.12	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381996&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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