Diglycolic acid, di(2-bromo-4-fluorophenyl) ester

Inchi: InChI=1S/C16H10Br2F2O5/c17-11-5-9(19)1-3-13(11)24-15(21)7-23-8-16(22)25-14-4-2-1

InchiKey: NIFJDLHXGABPDV-UHFFFAOYSA-N

Formula: C16H10Br2F2O5

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

Mol. weight [g/mol]: 480.05

Physical Properties

Property code	Value	Unit	Source
gf	-663.68	kJ/mol	Joback Method
hf	-907.77	kJ/mol	Joback Method
hfus	47.21	kJ/mol	Joback Method
hvap	90.37	kJ/mol	Joback Method
log10ws	-5.82		Crippen Method
logp	4.017		Crippen Method
mcvol	248.070	ml/mol	McGowan Method
pc	2429.05	kPa	Joback Method
rinpol	3472.00		NIST Webbook
rinpol	3472.00		NIST Webbook
tb	944.62	K	Joback Method
tc	1182.67	K	Joback Method
tf	660.33	K	Joback Method
vc	0.942	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	650.70	J/mol×K	944.62	Joback Method
cpg	658.59	J/mol×K	984.30	Joback Method
cpg	665.33	J/mol×K	1023.97	Joback Method
cpg	670.93	J/mol×K	1063.65	Joback Method
cpg	675.40	J/mol×K	1103.32	Joback Method
cpg	678.76	J/mol×K	1143.00	Joback Method
cpg	681.01	J/mol×K	1182.67	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382002&Units=SI

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