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

Inchi: InChI=1S/C20H28BrFO5/c1-2-3-4-5-6-7-8-9-12-26-19(23)14-25-15-20(24)27-18-11-10-1

InchiKey: SCCPKCZXBQMRNR-UHFFFAOYSA-N

Formula: C20H28BrFO5

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

Mol. weight [g/mol]: 447.34

Physical Properties

Property code	Value	Unit	Source
gf	-542.66	kJ/mol	Joback Method
hf	-1034.14	kJ/mol	Joback Method
hfus	55.95	kJ/mol	Joback Method
hvap	90.05	kJ/mol	Joback Method
log10ws	-6.25		Crippen Method
logp	5.194		Crippen Method
mcvol	308.920	ml/mol	McGowan Method
pc	1333.93	kPa	Joback Method
rinpol	3550.00		NIST Webbook
rinpol	3550.00		NIST Webbook
tb	934.07	K	Joback Method
tc	1146.06	K	Joback Method
tf	593.56	K	Joback Method
vc	1.194	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	952.14	J/mol×K	934.07	Joback Method
cpg	965.59	J/mol×K	969.40	Joback Method
cpg	977.78	J/mol×K	1004.73	Joback Method
cpg	988.73	J/mol×K	1040.07	Joback Method
cpg	998.44	J/mol×K	1075.40	Joback Method
cpg	1006.94	J/mol×K	1110.73	Joback Method
cpg	1014.25	J/mol×K	1146.06	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=U382001&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

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