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

Inchi: InChI=1S/C19H26BrFO5/c1-2-3-4-5-6-7-8-11-25-18(22)13-24-14-19(23)26-17-10-9-15(2

InchiKey: JQBIAICMGNDDRF-UHFFFAOYSA-N

Formula: C19H26BrFO5

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

Mol. weight [g/mol]: 433.31

Physical Properties

Property code	Value	Unit	Source
gf	-551.08	kJ/mol	Joback Method
hf	-1013.50	kJ/mol	Joback Method
hfus	53.36	kJ/mol	Joback Method
hvap	87.83	kJ/mol	Joback Method
log10ws	-5.83		Crippen Method
logp	4.804		Crippen Method
mcvol	294.830	ml/mol	McGowan Method
pc	1432.63	kPa	Joback Method
rinpol	3434.00		NIST Webbook
rinpol	3434.00		NIST Webbook
tb	911.19	K	Joback Method
tc	1120.67	K	Joback Method
tf	582.29	K	Joback Method
vc	1.137	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	893.26	J/mol×K	911.19	Joback Method
cpg	906.51	J/mol×K	946.10	Joback Method
cpg	918.57	J/mol×K	981.02	Joback Method
cpg	929.45	J/mol×K	1015.93	Joback Method
cpg	939.16	J/mol×K	1050.85	Joback Method
cpg	947.72	J/mol×K	1085.76	Joback Method
cpg	955.14	J/mol×K	1120.67	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382000&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

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