Succinic acid, dodec-2-en-1-yl 2-bromo-4-fluorophenyl ester

Inchi: InChI=1S/C22H30BrFO4/c1-2-3-4-5-6-7-8-9-10-11-16-27-21(25)14-15-22(26)28-20-13-12-17(24)16-18(20)23

InchiKey: OHHLCBZLFMSSKQ-ZHACJKMWSA-N

Formula: C22H30BrFO4

SMILES: CCCCCCCCCC=CCOC(=O)CCC(=O)Oc1ccc(F)cc1Br

Mol. weight [g/mol]: 457.37

Physical Properties

Property code	Value	Unit	Source
gf	-340.60	kJ/mol	Joback Method
hf	-825.98	kJ/mol	Joback Method
hfus	60.14	kJ/mol	Joback Method
hvap	92.05	kJ/mol	Joback Method
log10ws	-7.86		Crippen Method
logp	6.514		Crippen Method
mcvol	326.930	ml/mol	McGowan Method
pc	1221.70	kPa	Joback Method
rinpol	2908.00		NIST Webbook
tb	961.57	K	Joback Method
tc	1178.82	K	Joback Method
tf	588.79	K	Joback Method
vc	1.268	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1015.23	J/mol×K	961.57	Joback Method
cpg	1029.48	J/mol×K	997.78	Joback Method
cpg	1042.62	J/mol×K	1033.99	Joback Method
cpg	1054.69	J/mol×K	1070.20	Joback Method
cpg	1065.74	J/mol×K	1106.40	Joback Method
cpg	1075.84	J/mol×K	1142.61	Joback Method
cpg	1085.03	J/mol×K	1178.82	Joback Method

Sources

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=U389777&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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