Succinic acid, 2,2-dichloroethyl 2-bromo-4-fluorophenyl ester

Inchi: InChI=1S/C12H10BrCl2FO4/c13-8-5-7(16)1-2-9(8)20-12(18)4-3-11(17)19-6-10(14)15/h1-

InchiKey: GREPBZAYKWAYLJ-UHFFFAOYSA-N

Formula: C12H10BrCl2FO4

SMILES: O=C(CCC(=O)Oc1ccc(F)cc1Br)OCC(Cl)Cl

Mol. weight [g/mol]: 388.01

Physical Properties

Property code	Value	Unit	Source
gf	-531.32	kJ/mol	Joback Method
hf	-773.56	kJ/mol	Joback Method
hfus	38.91	kJ/mol	Joback Method
hvap	78.22	kJ/mol	Joback Method
log10ws	-4.73		Crippen Method
logp	3.621		Crippen Method
mcvol	214.810	ml/mol	McGowan Method
pc	2453.17	kPa	Joback Method
rinpol	2234.00		NIST Webbook
tb	803.03	K	Joback Method
tc	1027.06	K	Joback Method
tf	526.01	K	Joback Method
vc	0.820	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.78	J/mol×K	803.03	Joback Method
cpg	531.21	J/mol×K	840.37	Joback Method
cpg	539.79	J/mol×K	877.71	Joback Method
cpg	547.53	J/mol×K	915.04	Joback Method
cpg	554.44	J/mol×K	952.38	Joback Method
cpg	560.54	J/mol×K	989.72	Joback Method
cpg	565.82	J/mol×K	1027.06	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=U389767&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