Succinic acid, 2,4,6-trichlorophenyl 2-bromo-4-fluorophenyl ester

Inchi: InChI=1S/C16H9BrCl3FO4/c17-10-7-9(21)1-2-13(10)24-14(22)3-4-15(23)25-16-11(19)5-

InchiKey: MNKBBVQYDMBBPE-UHFFFAOYSA-N

Formula: C16H9BrCl3FO4

SMILES: O=C(CCC(=O)Oc1c(Cl)cc(Cl)cc1Cl)Oc1ccc(F)cc1Br

Mol. weight [g/mol]: 470.50

Physical Properties

Property code	Value	Unit	Source
gf	-423.61	kJ/mol	Joback Method
hf	-664.46	kJ/mol	Joback Method
hfus	49.86	kJ/mol	Joback Method
hvap	96.16	kJ/mol	Joback Method
log10ws	-7.30		Crippen Method
logp	5.840		Crippen Method
mcvol	259.650	ml/mol	McGowan Method
pc	2139.38	kPa	Joback Method
rinpol	2882.00		NIST Webbook
rinpol	2882.00		NIST Webbook
tb	974.04	K	Joback Method
tc	1221.01	K	Joback Method
tf	679.99	K	Joback Method
vc	0.991	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	644.05	J/mol×K	974.04	Joback Method
cpg	650.94	J/mol×K	1015.20	Joback Method
cpg	656.72	J/mol×K	1056.36	Joback Method
cpg	661.41	J/mol×K	1097.52	Joback Method
cpg	665.03	J/mol×K	1138.69	Joback Method
cpg	667.60	J/mol×K	1179.85	Joback Method
cpg	669.14	J/mol×K	1221.01	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=U389776&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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