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

Inchi: InChI=1S/C16H10BrClF2O4/c17-10-8-9(19)4-5-13(10)23-14(21)6-7-15(22)24-16-11(18)2

InchiKey: CPTOCYAQDGRLAI-UHFFFAOYSA-N

Formula: C16H10BrClF2O4

SMILES: O=C(CCC(=O)Oc1c(F)cccc1Cl)Oc1ccc(F)cc1Br

Mol. weight [g/mol]: 419.60

Physical Properties

Property code	Value	Unit	Source
gf	-584.93	kJ/mol	Joback Method
hf	-817.62	kJ/mol	Joback Method
hfus	44.94	kJ/mol	Joback Method
hvap	85.91	kJ/mol	Joback Method
log10ws	-6.26		Crippen Method
logp	4.672		Crippen Method
mcvol	236.940	ml/mol	McGowan Method
pc	2229.20	kPa	Joback Method
rinpol	2536.00		NIST Webbook
tb	893.47	K	Joback Method
tc	1126.61	K	Joback Method
tf	608.22	K	Joback Method
vc	0.910	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	619.72	J/mol×K	893.47	Joback Method
cpg	628.78	J/mol×K	932.33	Joback Method
cpg	636.81	J/mol×K	971.18	Joback Method
cpg	643.80	J/mol×K	1010.04	Joback Method
cpg	649.80	J/mol×K	1048.90	Joback Method
cpg	654.81	J/mol×K	1087.75	Joback Method
cpg	658.85	J/mol×K	1126.61	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=U389770&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

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