Succinic acid, di(2-chloro-6-fluorobenzyl) ester

Inchi: InChI=1S/C18H14Cl2F2O4/c19-13-3-1-5-15(21)11(13)9-25-17(23)7-8-18(24)26-10-12-14

InchiKey: BEZRVXNUAWATQV-UHFFFAOYSA-N

Formula: C18H14Cl2F2O4

SMILES: O=C(CCC(=O)OCc1c(F)cccc1Cl)OCc1c(F)cccc1Cl

Mol. weight [g/mol]: 403.20

Physical Properties

Property code	Value	Unit	Source
gf	-594.34	kJ/mol	Joback Method
hf	-900.97	kJ/mol	Joback Method
hfus	49.03	kJ/mol	Joback Method
hvap	88.31	kJ/mol	Joback Method
log10ws	-6.31		Crippen Method
logp	4.838		Crippen Method
mcvol	259.860	ml/mol	McGowan Method
pc	1713.19	kPa	Joback Method
rinpol	2728.00		NIST Webbook
rinpol	2728.00		NIST Webbook
tb	910.50	K	Joback Method
tc	1134.41	K	Joback Method
tf	600.88	K	Joback Method
vc	1.010	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	722.21	J/mol×K	910.50	Joback Method
cpg	732.28	J/mol×K	947.82	Joback Method
cpg	741.22	J/mol×K	985.14	Joback Method
cpg	749.05	J/mol×K	1022.45	Joback Method
cpg	755.80	J/mol×K	1059.77	Joback Method
cpg	761.46	J/mol×K	1097.09	Joback Method
cpg	766.07	J/mol×K	1134.41	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380873&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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