Succinic acid, 2-chloro-6-fluorobenzyl heptyl ester

Inchi: InChI=1S/C18H24ClFO4/c1-2-3-4-5-6-12-23-17(21)10-11-18(22)24-13-14-15(19)8-7-9-1

InchiKey: XEQFKLYSCHJULR-UHFFFAOYSA-N

Formula: C18H24ClFO4

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

Mol. weight [g/mol]: 358.83

Physical Properties

Property code	Value	Unit	Source
gf	-480.75	kJ/mol	Joback Method
hf	-902.71	kJ/mol	Joback Method
hfus	48.49	kJ/mol	Joback Method
hvap	81.14	kJ/mol	Joback Method
log10ws	-5.70		Crippen Method
logp	4.816		Crippen Method
mcvol	269.610	ml/mol	McGowan Method
pc	1440.25	kPa	Joback Method
rinpol	2414.00		NIST Webbook
rinpol	2414.00		NIST Webbook
tb	837.16	K	Joback Method
tc	1037.52	K	Joback Method
tf	518.91	K	Joback Method
vc	1.050	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	794.89	J/mol×K	837.16	Joback Method
cpg	808.91	J/mol×K	870.55	Joback Method
cpg	821.91	J/mol×K	903.95	Joback Method
cpg	833.90	J/mol×K	937.34	Joback Method
cpg	844.90	J/mol×K	970.73	Joback Method
cpg	854.92	J/mol×K	1004.13	Joback Method
cpg	863.98	J/mol×K	1037.52	Joback Method

Sources

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=U380864&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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