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

Inchi: InChI=1S/C16H20ClFO4/c1-2-3-4-10-21-15(19)8-9-16(20)22-11-12-13(17)6-5-7-14(12)18

InchiKey: OFZNTPDIEBBGGD-UHFFFAOYSA-N

Formula: C16H20ClFO4

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

Mol. weight [g/mol]: 330.78

Physical Properties

Property code	Value	Unit	Source
gf	-497.59	kJ/mol	Joback Method
hf	-861.43	kJ/mol	Joback Method
hfus	43.31	kJ/mol	Joback Method
hvap	76.69	kJ/mol	Joback Method
log10ws	-4.86		Crippen Method
logp	4.036		Crippen Method
mcvol	241.430	ml/mol	McGowan Method
pc	1675.53	kPa	Joback Method
rinpol	2217.00		NIST Webbook
rinpol	2217.00		NIST Webbook
tb	791.40	K	Joback Method
tc	991.82	K	Joback Method
tf	496.37	K	Joback Method
vc	0.939	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	681.78	J/mol×K	791.40	Joback Method
cpg	695.20	J/mol×K	824.80	Joback Method
cpg	707.70	J/mol×K	858.21	Joback Method
cpg	719.26	J/mol×K	891.61	Joback Method
cpg	729.92	J/mol×K	925.01	Joback Method
cpg	739.67	J/mol×K	958.42	Joback Method
cpg	748.52	J/mol×K	991.82	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=U380861&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