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

Inchi: InChI=1S/C15H18ClFO4/c1-2-3-9-20-14(18)7-8-15(19)21-10-11-12(16)5-4-6-13(11)17/h4

InchiKey: PYIPJBZLBSVXRJ-UHFFFAOYSA-N

Formula: C15H18ClFO4

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

Mol. weight [g/mol]: 316.75

Physical Properties

Property code	Value	Unit	Source
gf	-506.01	kJ/mol	Joback Method
hf	-840.79	kJ/mol	Joback Method
hfus	40.72	kJ/mol	Joback Method
hvap	74.46	kJ/mol	Joback Method
log10ws	-4.44		Crippen Method
logp	3.646		Crippen Method
mcvol	227.340	ml/mol	McGowan Method
pc	1815.41	kPa	Joback Method
rinpol	2113.00		NIST Webbook
rinpol	2113.00		NIST Webbook
tb	768.52	K	Joback Method
tc	969.89	K	Joback Method
tf	485.10	K	Joback Method
vc	0.882	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	626.67	J/mol×K	768.52	Joback Method
cpg	639.75	J/mol×K	802.08	Joback Method
cpg	651.93	J/mol×K	835.64	Joback Method
cpg	663.23	J/mol×K	869.21	Joback Method
cpg	673.65	J/mol×K	902.77	Joback Method
cpg	683.20	J/mol×K	936.33	Joback Method
cpg	691.90	J/mol×K	969.89	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380860&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