Succinic acid, isobutyl 2,3,4,5-tetrafluorobenzyl ester

Inchi: InChI=1S/C15H16F4O4/c1-8(2)6-22-11(20)3-4-12(21)23-7-9-5-10(16)14(18)15(19)13(9)1

InchiKey: PGRVKLZCUDUNJO-UHFFFAOYSA-N

Formula: C15H16F4O4

SMILES: CC(C)COC(=O)CCC(=O)OCc1cc(F)c(F)c(F)c1F

Mol. weight [g/mol]: 336.28

Physical Properties

Property code	Value	Unit	Source
gf	-1100.21	kJ/mol	Joback Method
hf	-1441.60	kJ/mol	Joback Method
hfus	41.46	kJ/mol	Joback Method
hvap	68.56	kJ/mol	Joback Method
log10ws	-4.51		Crippen Method
logp	3.266		Crippen Method
mcvol	220.410	ml/mol	McGowan Method
pc	1643.09	kPa	Joback Method
rinpol	1807.00		NIST Webbook
rinpol	1807.00		NIST Webbook
tb	738.42	K	Joback Method
tc	922.72	K	Joback Method
tf	466.99	K	Joback Method
vc	0.881	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	622.65	J/mol×K	738.42	Joback Method
cpg	635.29	J/mol×K	769.14	Joback Method
cpg	647.19	J/mol×K	799.85	Joback Method
cpg	658.34	J/mol×K	830.57	Joback Method
cpg	668.74	J/mol×K	861.28	Joback Method
cpg	678.40	J/mol×K	892.00	Joback Method
cpg	687.30	J/mol×K	922.72	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381612&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