Succinic acid, 2,5-difluorobenzyl 2-methylhex-3-yl ester

Inchi: InChI=1S/C18H24F2O4/c1-4-5-16(12(2)3)24-18(22)9-8-17(21)23-11-13-10-14(19)6-7-15

InchiKey: HZKAPFBYJABPKZ-UHFFFAOYSA-N

Formula: C18H24F2O4

SMILES: CCCC(OC(=O)CCC(=O)OCc1cc(F)ccc1F)C(C)C

Mol. weight [g/mol]: 342.38

Physical Properties

Property code	Value	Unit	Source
gf	-668.51	kJ/mol	Joback Method
hf	-1093.64	kJ/mol	Joback Method
hfus	40.33	kJ/mol	Joback Method
hvap	75.16	kJ/mol	Joback Method
log10ws	-5.21		Crippen Method
logp	4.156		Crippen Method
mcvol	259.140	ml/mol	McGowan Method
pc	1449.04	kPa	Joback Method
rinpol	2069.00		NIST Webbook
rinpol	2069.00		NIST Webbook
tb	798.12	K	Joback Method
tc	992.81	K	Joback Method
tf	459.58	K	Joback Method
vc	1.008	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	776.69	J/mol×K	798.12	Joback Method
cpg	791.64	J/mol×K	830.57	Joback Method
cpg	805.59	J/mol×K	863.02	Joback Method
cpg	818.54	J/mol×K	895.46	Joback Method
cpg	830.50	J/mol×K	927.91	Joback Method
cpg	841.49	J/mol×K	960.36	Joback Method
cpg	851.52	J/mol×K	992.81	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381221&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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