Succinic acid, di(3,4-difluorobenzyl) ester

Inchi: InChI=1S/C18H14F4O4/c19-13-3-1-11(7-15(13)21)9-25-17(23)5-6-18(24)26-10-12-2-4-14(20)16(22)8-12/h1-4,7-8H,5-6,9-10H2

InchiKey: VRKNQIUJMKCTIJ-UHFFFAOYSA-N

Formula: C18H14F4O4

SMILES: O=C(CCC(=O)OCc1ccc(F)c(F)c1)OCc1ccc(F)c(F)c1

Mol. weight [g/mol]: 370.30

Physical Properties

Property code	Value	Unit	Source
gf	-960.10	kJ/mol	Joback Method
hf	-1261.71	kJ/mol	Joback Method
hfus	46.80	kJ/mol	Joback Method
hvap	77.91	kJ/mol	Joback Method
log10ws	-5.61		Crippen Method
logp	3.810		Crippen Method
mcvol	238.920	ml/mol	McGowan Method
pc	1690.72	kPa	Joback Method
rinpol	2321.00		NIST Webbook
rinpol	2321.00		NIST Webbook
tb	834.18	K	Joback Method
tc	1038.95	K	Joback Method
tf	542.22	K	Joback Method
vc	0.948	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	694.39	J/mol×K	834.18	Joback Method
cpg	706.11	J/mol×K	868.31	Joback Method
cpg	716.82	J/mol×K	902.44	Joback Method
cpg	726.56	J/mol×K	936.57	Joback Method
cpg	735.32	J/mol×K	970.69	Joback Method
cpg	743.12	J/mol×K	1004.82	Joback Method
cpg	749.97	J/mol×K	1038.95	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381755&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

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