Succinic acid, 2,5-difluorobenzyl ethyl ester

Inchi: InChI=1S/C13H14F2O4/c1-2-18-12(16)5-6-13(17)19-8-9-7-10(14)3-4-11(9)15/h3-4,7H,2,
InchiKey: XDBVGUZHWZZBPV-UHFFFAOYSA-N
Formula: C13H14F2O4
SMILES: CCOC(=O)CCC(=O)OCc1cc(F)ccc1F
Mol. weight [g/mol]: 272.24

Physical Properties

Property code	Value	Unit	Source
gf	-705.73	kJ/mol	Joback Method
hf	-979.88	kJ/mol	Joback Method
hfus	34.42	kJ/mol	Joback Method
hvap	64.81	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	2.351		Crippen Method
mcvol	188.690	ml/mol	McGowan Method
pc	2137.41	kPa	Joback Method
rinpol	1717.00		NIST Webbook
rinpol	1717.00		NIST Webbook
tb	684.60	K	Joback Method
tc	878.41	K	Joback Method
tf	433.23	K	Joback Method
vc	0.740	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	502.56	J/mol×K	684.60	Joback Method
cpg	515.16	J/mol×K	716.90	Joback Method
cpg	527.04	J/mol×K	749.20	Joback Method
cpg	538.19	J/mol×K	781.50	Joback Method
cpg	548.61	J/mol×K	813.81	Joback Method
cpg	558.31	J/mol×K	846.11	Joback Method
cpg	567.28	J/mol×K	878.41	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381217&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