

Succinic acid, di(3-fluorobenzyl) ester

Inchi:	InChI=1S/C18H16F2O4/c19-15-5-1-3-13(9-15)11-23-17(21)7-8-18(22)24-12-14-4-2-6-16
InchiKey:	APENLMGYKZZEB-UHFFFAOYSA-N
Formula:	C18H16F2O4
SMILES:	O=C(CCC(=O)OCc1cccc(F)c1)OCc1cccc(F)c1
Mol. weight [g/mol]:	334.31

Physical Properties

Property code	Value	Unit	Source
gf	-551.22	kJ/mol	Joback Method
hf	-846.55	kJ/mol	Joback Method
hfus	41.41	kJ/mol	Joback Method
hvap	78.22	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	3.532		Crippen Method
mvol	235.380	ml/mol	McGowan Method
pc	1870.79	kPa	Joback Method
rinpol	2275.00		NIST Webbook
rinpol	2275.00		NIST Webbook
tb	825.68	K	Joback Method
tc	1040.41	K	Joback Method
tf	516.00	K	Joback Method
vc	0.911	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	681.99	J/molxK	825.68	Joback Method
cpg	694.76	J/molxK	861.47	Joback Method
cpg	706.42	J/molxK	897.26	Joback Method
cpg	717.01	J/molxK	933.04	Joback Method
cpg	726.55	J/molxK	968.83	Joback Method
cpg	735.06	J/molxK	1004.62	Joback Method
cpg	742.55	J/molxK	1040.41	Joback Method

Sources

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=U381249&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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