

Succinic acid, 2,4,5-trifluorobenzyl undecyl ester

Inchi:	InChI=1S/C22H31F3O4/c1-2-3-4-5-6-7-8-9-10-13-28-21(26)11-12-22(27)29-16-17-14-19
InchiKey:	DLESREKYSZAHAN-UHFFFAOYSA-N
Formula:	C22H31F3O4
SMILES:	CCCCCCCCCOC(=O)CCC(=O)OCc1cc(F)c(F)cc1F
Mol. weight [g/mol]:	416.47

Physical Properties

Property code	Value	Unit	Source
gf	-834.39	kJ/mol	Joback Method
hf	-1373.22	kJ/mol	Joback Method
hfus	60.42	kJ/mol	Joback Method
hvap	84.69	kJ/mol	Joback Method
log10ws	-7.35		Crippen Method
logp	6.001		Crippen Method
mvol	317.270	ml/mol	McGowan Method
pc	1049.37	kPa	Joback Method
rinpol	2564.00		NIST Webbook
rinpol	2564.00		NIST Webbook
tb	894.77	K	Joback Method
tc	1095.50	K	Joback Method
tf	547.77	K	Joback Method
vc	1.262	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1017.57	J/molxK	894.77	Joback Method
cpg	1033.28	J/molxK	928.23	Joback Method
cpg	1047.78	J/molxK	961.68	Joback Method
cpg	1061.10	J/molxK	995.14	Joback Method
cpg	1073.24	J/molxK	1028.59	Joback Method
cpg	1084.23	J/molxK	1062.05	Joback Method
cpg	1094.09	J/molxK	1095.50	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=U382226&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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