Succinic acid, dodecyl 2-fluoro-6-(trifluoromethyl)benzyl ester

Inchi: InChI=1S/C24H34F4O4/c1-2-3-4-5-6-7-8-9-10-11-17-31-22(29)15-16-23(30)32-18-19-20

InchiKey: DYEXYSWMYODUGW-UHFFFAOYSA-N

Formula: C24H34F4O4

SMILES: CCCCCCCCCCCCOC(=O)CCC(=O)OCc1c(F)cccc1C(F)(F)F

Mol. weight [g/mol]: 462.52

Physical Properties

Property code	Value	Unit	Source
gf	-999.89	kJ/mol	Joback Method
hf	-1607.89	kJ/mol	Joback Method
hfus	61.66	kJ/mol	Joback Method
hvap	86.37	kJ/mol	Joback Method
log10ws	-8.21		Crippen Method
logp	7.132		Crippen Method
mcvol	347.220	ml/mol	McGowan Method
pc	923.86	kPa	Joback Method
rinpol	2708.00		NIST Webbook
rinpol	2708.00		NIST Webbook
tb	931.59	K	Joback Method
tc	1141.36	K	Joback Method
tf	560.80	K	Joback Method
vc	1.381	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1147.01	J/mol×K	931.59	Joback Method
cpg	1163.31	J/mol×K	966.55	Joback Method
cpg	1178.32	J/mol×K	1001.51	Joback Method
cpg	1192.09	J/mol×K	1036.47	Joback Method
cpg	1204.68	J/mol×K	1071.44	Joback Method
cpg	1216.14	J/mol×K	1106.40	Joback Method
cpg	1226.54	J/mol×K	1141.36	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=U381642&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