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

Inchi: InChI=1S/C19H24F4O4/c1-2-3-4-5-6-12-26-17(24)10-11-18(25)27-13-14-15(19(21,22)23
InchiKey: DYXBXSSGCGLSTQ-UHFFFAOYSA-N
Formula: C19H24F4O4
SMILES: CCCCCCCOC(=O)CCC(=O)OCc1c(F)cccc1C(F)(F)F
Mol. weight [g/mol]: 392.39

Physical Properties

Property code	Value	Unit	Source
gf	-1041.99	kJ/mol	Joback Method
hf	-1504.69	kJ/mol	Joback Method
hfus	48.71	kJ/mol	Joback Method
hvap	75.24	kJ/mol	Joback Method
log10ws	-6.12		Crippen Method
logp	5.182		Crippen Method
mcvol	276.770	ml/mol	McGowan Method
pc	1266.45	kPa	Joback Method
rinpol	2216.00		NIST Webbook
rinpol	2216.00		NIST Webbook
tb	817.19	K	Joback Method
tc	1006.53	K	Joback Method
tf	504.45	K	Joback Method
vc	1.101	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	849.51	J/mol×K	817.19	Joback Method
cpg	863.86	J/mol×K	848.75	Joback Method
cpg	877.24	J/mol×K	880.30	Joback Method
cpg	889.68	J/mol×K	911.86	Joback Method
cpg	901.22	J/mol×K	943.41	Joback Method
cpg	911.88	J/mol×K	974.97	Joback Method
cpg	921.70	J/mol×K	1006.53	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381637&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