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

Inchi: InChI=1S/C17H20F4O4/c1-2-3-4-10-24-15(22)8-9-16(23)25-11-12-13(17(19,20)21)6-5-7

InchiKey: GHLPVZJYBKGAJE-UHFFFAOYSA-N

Formula: C17H20F4O4

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

Mol. weight [g/mol]: 364.33

Physical Properties

Property code	Value	Unit	Source
gf	-1058.83	kJ/mol	Joback Method
hf	-1463.41	kJ/mol	Joback Method
hfus	43.53	kJ/mol	Joback Method
hvap	70.78	kJ/mol	Joback Method
log10ws	-5.28		Crippen Method
logp	4.401		Crippen Method
mcvol	248.590	ml/mol	McGowan Method
pc	1459.02	kPa	Joback Method
rinpol	2018.00		NIST Webbook
rinpol	2018.00		NIST Webbook
tb	771.43	K	Joback Method
tc	958.10	K	Joback Method
tf	481.91	K	Joback Method
vc	0.989	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	736.00	J/mol×K	771.43	Joback Method
cpg	749.63	J/mol×K	802.54	Joback Method
cpg	762.37	J/mol×K	833.65	Joback Method
cpg	774.25	J/mol×K	864.77	Joback Method
cpg	785.31	J/mol×K	895.88	Joback Method
cpg	795.55	J/mol×K	926.99	Joback Method
cpg	805.01	J/mol×K	958.10	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381634&Units=SI

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