Succinic acid, hexyl 4-trifluoromethoxybenzyl ester

Inchi: InChI=1S/C18H23F3O5/c1-2-3-4-5-12-24-16(22)10-11-17(23)25-13-14-6-8-15(9-7-14)26

InchiKey: JPZFWVIYAPKCAN-UHFFFAOYSA-N

Formula: C18H23F3O5

SMILES: CCCCCCOC(=O)CCC(=O)OCc1ccc(OC(F)(F)F)cc1

Mol. weight [g/mol]: 376.37

Physical Properties

Property code	Value	Unit	Source
gf	-950.97	kJ/mol	Joback Method
hf	-1408.69	kJ/mol	Joback Method
hfus	44.62	kJ/mol	Joback Method
hvap	75.58	kJ/mol	Joback Method
log10ws	-5.54		Crippen Method
logp	4.532		Crippen Method
mcvol	266.780	ml/mol	McGowan Method
pc	1401.69	kPa	Joback Method
rinpol	2110.00		NIST Webbook
rinpol	2110.00		NIST Webbook
tb	812.48	K	Joback Method
tc	1004.53	K	Joback Method
tf	502.30	K	Joback Method
vc	1.044	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	813.86	J/mol×K	812.48	Joback Method
cpg	827.98	J/mol×K	844.49	Joback Method
cpg	841.09	J/mol×K	876.50	Joback Method
cpg	853.21	J/mol×K	908.51	Joback Method
cpg	864.37	J/mol×K	940.52	Joback Method
cpg	874.59	J/mol×K	972.52	Joback Method
cpg	883.88	J/mol×K	1004.53	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381565&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