Succinic acid, pentyl 4-trifluoromethoxybenzyl ester

Inchi: InChI=1S/C17H21F3O5/c1-2-3-4-11-23-15(21)9-10-16(22)24-12-13-5-7-14(8-6-13)25-17(18,19)20/h5-8H,2-4,9-12H2,1H3

InchiKey: HLBFVQWKJJOFDW-UHFFFAOYSA-N

Formula: C17H21F3O5

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

Mol. weight [g/mol]: 362.34

Physical Properties

Property code	Value	Unit	Source
gf	-959.39	kJ/mol	Joback Method
hf	-1388.05	kJ/mol	Joback Method
hfus	42.03	kJ/mol	Joback Method
hvap	73.35	kJ/mol	Joback Method
log10ws	-5.12		Crippen Method
logp	4.142		Crippen Method
mcvol	252.690	ml/mol	McGowan Method
pc	1508.15	kPa	Joback Method
rinpol	2012.00		NIST Webbook
rinpol	2012.00		NIST Webbook
tb	789.60	K	Joback Method
tc	980.78	K	Joback Method
tf	491.03	K	Joback Method
vc	0.989	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	757.10	J/mol×K	789.60	Joback Method
cpg	770.91	J/mol×K	821.46	Joback Method
cpg	783.76	J/mol×K	853.33	Joback Method
cpg	795.66	J/mol×K	885.19	Joback Method
cpg	806.64	J/mol×K	917.05	Joback Method
cpg	816.72	J/mol×K	948.91	Joback Method
cpg	825.91	J/mol×K	980.78	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381563&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