Succinic acid, nonyl 4-trifluoromethylbenzyl ester

Inchi: InChI=1S/C21H29F3O4/c1-2-3-4-5-6-7-8-15-27-19(25)13-14-20(26)28-16-17-9-11-18(12

InchiKey: ZANWCLYPJSLBDQ-UHFFFAOYSA-N

Formula: C21H29F3O4

SMILES: CCCCCCCCCOC(=O)CCC(=O)OCc1ccc(C(F)(F)F)cc1

Mol. weight [g/mol]: 402.45

Physical Properties

Property code	Value	Unit	Source
gf	-820.71	kJ/mol	Joback Method
hf	-1338.39	kJ/mol	Joback Method
hfus	51.20	kJ/mol	Joback Method
hvap	79.84	kJ/mol	Joback Method
log10ws	-6.62		Crippen Method
logp	5.823		Crippen Method
mcvol	303.180	ml/mol	McGowan Method
pc	1155.35	kPa	Joback Method
rinpol	2408.00		NIST Webbook
rinpol	2408.00		NIST Webbook
tb	858.70	K	Joback Method
tc	1054.45	K	Joback Method
tf	513.88	K	Joback Method
vc	1.194	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	959.81	J/mol×K	858.70	Joback Method
cpg	975.20	J/mol×K	891.33	Joback Method
cpg	989.51	J/mol×K	923.95	Joback Method
cpg	1002.78	J/mol×K	956.58	Joback Method
cpg	1015.04	J/mol×K	989.20	Joback Method
cpg	1026.35	J/mol×K	1021.83	Joback Method
cpg	1036.75	J/mol×K	1054.45	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382446&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