Succinic acid, ethyl 1-phenyl-2,2,2-trifluoroethyl ester

Inchi: InChI=1S/C14H15F3O4/c1-2-20-11(18)8-9-12(19)21-13(14(15,16)17)10-6-4-3-5-7-10/h3-

InchiKey: NSKMJTGLDUGMLP-UHFFFAOYSA-N

Formula: C14H15F3O4

SMILES: CCOC(=O)CCC(=O)OC(c1ccccc1)C(F)(F)F

Mol. weight [g/mol]: 304.26

Physical Properties

Property code	Value	Unit	Source
gf	-872.46	kJ/mol	Joback Method
hf	-1187.72	kJ/mol	Joback Method
hfus	29.93	kJ/mol	Joback Method
hvap	63.21	kJ/mol	Joback Method
log10ws	-3.63		Crippen Method
logp	3.176		Crippen Method
mcvol	204.550	ml/mol	McGowan Method
pc	1980.59	kPa	Joback Method
rinpol	1623.00		NIST Webbook
rinpol	1623.00		NIST Webbook
tb	693.12	K	Joback Method
tc	887.98	K	Joback Method
tf	407.47	K	Joback Method
vc	0.796	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	567.86	J/mol×K	693.12	Joback Method
cpg	581.24	J/mol×K	725.60	Joback Method
cpg	593.73	J/mol×K	758.07	Joback Method
cpg	605.34	J/mol×K	790.55	Joback Method
cpg	616.12	J/mol×K	823.03	Joback Method
cpg	626.08	J/mol×K	855.51	Joback Method
cpg	635.26	J/mol×K	887.98	Joback Method

Sources

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=U381567&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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