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

Inchi: InChI=1S/C16H19F3O4/c1-11(2)10-22-13(20)8-9-14(21)23-15(16(17,18)19)12-6-4-3-5-7

InchiKey: WZEDVLPXWVLITH-UHFFFAOYSA-N

Formula: C16H19F3O4

SMILES: CC(C)COC(=O)CCC(=O)OC(c1ccccc1)C(F)(F)F

Mol. weight [g/mol]: 332.31

Physical Properties

Property code	Value	Unit	Source
gf	-858.06	kJ/mol	Joback Method
hf	-1234.28	kJ/mol	Joback Method
hfus	31.59	kJ/mol	Joback Method
hvap	67.27	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	3.813		Crippen Method
mcvol	232.730	ml/mol	McGowan Method
pc	1692.12	kPa	Joback Method
rinpol	1760.00		NIST Webbook
rinpol	1760.00		NIST Webbook
tb	738.44	K	Joback Method
tc	933.27	K	Joback Method
tf	415.01	K	Joback Method
vc	0.902	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	675.77	J/mol×K	738.44	Joback Method
cpg	690.07	J/mol×K	770.91	Joback Method
cpg	703.39	J/mol×K	803.38	Joback Method
cpg	715.77	J/mol×K	835.86	Joback Method
cpg	727.23	J/mol×K	868.33	Joback Method
cpg	737.81	J/mol×K	900.80	Joback Method
cpg	747.55	J/mol×K	933.27	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=U381569&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