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

Inchi: InChI=1S/C19H25F3O4/c1-2-3-4-5-9-14-25-16(23)12-13-17(24)26-18(19(20,21)22)15-10

InchiKey: MAAHYWYPPRHNLT-UHFFFAOYSA-N

Formula: C19H25F3O4

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

Mol. weight [g/mol]: 374.39

Physical Properties

Property code	Value	Unit	Source
gf	-830.36	kJ/mol	Joback Method
hf	-1290.92	kJ/mol	Joback Method
hfus	42.88	kJ/mol	Joback Method
hvap	74.34	kJ/mol	Joback Method
log10ws	-5.73		Crippen Method
logp	5.127		Crippen Method
mcvol	275.000	ml/mol	McGowan Method
pc	1344.71	kPa	Joback Method
rinpol	2093.00		NIST Webbook
rinpol	2093.00		NIST Webbook
tb	807.52	K	Joback Method
tc	999.89	K	Joback Method
tf	463.82	K	Joback Method
vc	1.077	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	844.07	J/mol×K	807.52	Joback Method
cpg	859.03	J/mol×K	839.58	Joback Method
cpg	872.97	J/mol×K	871.64	Joback Method
cpg	885.93	J/mol×K	903.70	Joback Method
cpg	897.93	J/mol×K	935.77	Joback Method
cpg	909.03	J/mol×K	967.83	Joback Method
cpg	919.25	J/mol×K	999.89	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381574&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