Succinic acid, 1,1,1-trifluoroprop-2-yl 1-cyclopentylethyl ester

Inchi: InChI=1S/C14H21F3O4/c1-9(11-5-3-4-6-11)20-12(18)7-8-13(19)21-10(2)14(15,16)17/h9-
InchiKey: TXGJNSBWFOTQEU-UHFFFAOYSA-N
Formula: C14H21F3O4
SMILES: CC(OC(=O)CCC(=O)OC(C)C(F)(F)F)C1CCCC1
Mol. weight [g/mol]: 310.31

Physical Properties

Property code	Value	Unit	Source
gf	-950.76	kJ/mol	Joback Method
hf	-1369.05	kJ/mol	Joback Method
hfus	26.30	kJ/mol	Joback Method
hvap	60.80	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.383		Crippen Method
mcvol	217.450	ml/mol	McGowan Method
pc	1750.67	kPa	Joback Method
rinpol	1609.00		NIST Webbook
rinpol	1609.00		NIST Webbook
tb	681.28	K	Joback Method
tc	869.29	K	Joback Method
tf	376.95	K	Joback Method
vc	0.840	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	640.13	J/mol×K	681.28	Joback Method
cpg	656.45	J/mol×K	712.62	Joback Method
cpg	671.77	J/mol×K	743.95	Joback Method
cpg	686.14	J/mol×K	775.29	Joback Method
cpg	699.58	J/mol×K	806.62	Joback Method
cpg	712.12	J/mol×K	837.96	Joback Method
cpg	723.79	J/mol×K	869.29	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=U391406&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