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

Inchi: InChI=1S/C14H21F3O4/c1-10(14(15,16)17)21-13(19)8-7-12(18)20-9-11-5-3-2-4-6-11/h1

InchiKey: ZIFFLTWXCWVDSC-UHFFFAOYSA-N

Formula: C14H21F3O4

SMILES: CC(OC(=O)CCC(=O)OCC1CCCCC1)C(F)(F)F

Mol. weight [g/mol]: 310.31

Physical Properties

Property code	Value	Unit	Source
gf	-960.42	kJ/mol	Joback Method
hf	-1369.93	kJ/mol	Joback Method
hfus	27.73	kJ/mol	Joback Method
hvap	61.36	kJ/mol	Joback Method
log10ws	-3.84		Crippen Method
logp	3.384		Crippen Method
mcvol	217.450	ml/mol	McGowan Method
pc	1775.84	kPa	Joback Method
rinpol	1634.00		NIST Webbook
rinpol	1634.00		NIST Webbook
tb	685.99	K	Joback Method
tc	875.95	K	Joback Method
tf	388.43	K	Joback Method
vc	0.838	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	642.42	J/mol×K	685.99	Joback Method
cpg	659.08	J/mol×K	717.65	Joback Method
cpg	674.71	J/mol×K	749.31	Joback Method
cpg	689.33	J/mol×K	780.97	Joback Method
cpg	702.98	J/mol×K	812.63	Joback Method
cpg	715.67	J/mol×K	844.29	Joback Method
cpg	727.42	J/mol×K	875.95	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=U390844&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