Succinic acid, 1,1,1-trifluoroprop-2-yl cis-4-methylcyclohexyl ester

Inchi: InChI=1S/C14H21F3O4/c1-9-3-5-11(6-4-9)21-13(19)8-7-12(18)20-10(2)14(15,16)17/h9-1

InchiKey: KNYVTMOOHSPWOG-UHFFFAOYSA-N

Formula: C14H21F3O4

SMILES: CC1CCC(OC(=O)CCC(=O)OC(C)C(F)(F)F)CC1

Mol. weight [g/mol]: 310.31

Physical Properties

Property code	Value	Unit	Source
gf	-968.13	kJ/mol	Joback Method
hf	-1390.27	kJ/mol	Joback Method
hfus	28.80	kJ/mol	Joback Method
hvap	61.06	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.383		Crippen Method
mcvol	217.450	ml/mol	McGowan Method
pc	1727.46	kPa	Joback Method
rinpol	1584.00		NIST Webbook
rinpol	1584.00		NIST Webbook
tb	681.32	K	Joback Method
tc	871.06	K	Joback Method
tf	384.19	K	Joback Method
vc	0.837	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	644.56	J/mol×K	681.32	Joback Method
cpg	661.67	J/mol×K	712.94	Joback Method
cpg	677.73	J/mol×K	744.57	Joback Method
cpg	692.76	J/mol×K	776.19	Joback Method
cpg	706.80	J/mol×K	807.81	Joback Method
cpg	719.85	J/mol×K	839.44	Joback Method
cpg	731.93	J/mol×K	871.06	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390052&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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