Succinic acid, 2,2,3,3-tetrafluoropropyl 3,5-dimethylcyclohexyl ester

Inchi: InChI=1S/C15H22F4O4/c1-9-5-10(2)7-11(6-9)23-13(21)4-3-12(20)22-8-15(18,19)14(16)1

InchiKey: AZYZLRYWBGOYTN-UHFFFAOYSA-N

Formula: C15H22F4O4

SMILES: CC1CC(C)CC(OC(=O)CCC(=O)OCC(F)(F)C(F)F)C1

Mol. weight [g/mol]: 342.33

Physical Properties

Property code	Value	Unit	Source
gf	-1162.23	kJ/mol	Joback Method
hf	-1627.36	kJ/mol	Joback Method
hfus	35.54	kJ/mol	Joback Method
hvap	62.16	kJ/mol	Joback Method
log10ws	-3.98		Crippen Method
logp	3.578		Crippen Method
mcvol	233.310	ml/mol	McGowan Method
pc	1502.31	kPa	Joback Method
rinpol	1718.00		NIST Webbook
rinpol	1718.00		NIST Webbook
tb	698.80	K	Joback Method
tc	881.08	K	Joback Method
tf	391.81	K	Joback Method
vc	0.909	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	710.21	J/mol×K	698.80	Joback Method
cpg	727.38	J/mol×K	729.18	Joback Method
cpg	743.52	J/mol×K	759.56	Joback Method
cpg	758.66	J/mol×K	789.94	Joback Method
cpg	772.80	J/mol×K	820.32	Joback Method
cpg	785.96	J/mol×K	850.70	Joback Method
cpg	798.16	J/mol×K	881.08	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391389&Units=SI

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