Succinic acid, 2,2,3,3-tetrafluoropropyl 2,4,4-trimethylpentyl ester

Inchi: InChI=1S/C15H24F4O4/c1-10(7-14(2,3)4)8-22-11(20)5-6-12(21)23-9-15(18,19)13(16)17/

InchiKey: LEDHNTIUKHYGJA-UHFFFAOYSA-N

Formula: C15H24F4O4

SMILES: CC(COC(=O)CCC(=O)OCC(F)(F)C(F)F)CC(C)(C)C

Mol. weight [g/mol]: 344.34

Physical Properties

Property code	Value	Unit	Source
gf	-1170.86	kJ/mol	Joback Method
hf	-1655.03	kJ/mol	Joback Method
hfus	30.63	kJ/mol	Joback Method
hvap	60.66	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	3.826		Crippen Method
mcvol	244.170	ml/mol	McGowan Method
pc	1379.91	kPa	Joback Method
rinpol	1593.00		NIST Webbook
rinpol	1593.00		NIST Webbook
tb	684.92	K	Joback Method
tc	856.64	K	Joback Method
tf	380.33	K	Joback Method
vc	0.962	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	714.40	J/mol×K	684.92	Joback Method
cpg	729.61	J/mol×K	713.54	Joback Method
cpg	743.97	J/mol×K	742.16	Joback Method
cpg	757.54	J/mol×K	770.78	Joback Method
cpg	770.32	J/mol×K	799.40	Joback Method
cpg	782.36	J/mol×K	828.02	Joback Method
cpg	793.67	J/mol×K	856.64	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=U389540&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