Succinic acid, 1,1,1-trifluoroprop-2-yl 2,4,4-trimethylpentyl ester

Inchi: InChI=1S/C15H25F3O4/c1-10(8-14(3,4)5)9-21-12(19)6-7-13(20)22-11(2)15(16,17)18/h1

InchiKey: LKFDDPTVCISPQJ-UHFFFAOYSA-N

Formula: C15H25F3O4

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

Mol. weight [g/mol]: 326.35

Physical Properties

Property code	Value	Unit	Source
gf	-976.05	kJ/mol	Joback Method
hf	-1458.92	kJ/mol	Joback Method
hfus	27.55	kJ/mol	Joback Method
hvap	61.48	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	3.876		Crippen Method
mcvol	242.400	ml/mol	McGowan Method
pc	1427.22	kPa	Joback Method
rinpol	1503.00		NIST Webbook
rinpol	1503.00		NIST Webbook
tb	685.65	K	Joback Method
tc	862.33	K	Joback Method
tf	379.74	K	Joback Method
vc	0.944	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	706.54	J/mol×K	685.65	Joback Method
cpg	722.23	J/mol×K	715.10	Joback Method
cpg	737.05	J/mol×K	744.54	Joback Method
cpg	751.03	J/mol×K	773.99	Joback Method
cpg	764.19	J/mol×K	803.44	Joback Method
cpg	776.57	J/mol×K	832.89	Joback Method
cpg	788.19	J/mol×K	862.33	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=U389539&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