Succinic acid, octyl 2,2,2-trifluoroethyl ester

Inchi: InChI=1S/C14H23F3O4/c1-2-3-4-5-6-7-10-20-12(18)8-9-13(19)21-11-14(15,16)17/h2-11
InchiKey: SLHZKFYGRIBDDT-UHFFFAOYSA-N
Formula: C14H23F3O4
SMILES: CCCCCCCCOC(=O)CCC(=O)OCC(F)(F)F
Mol. weight [g/mol]: 312.33

Physical Properties

Property code	Value	Unit	Source
gf	-982.43	kJ/mol	Joback Method
hf	-1418.97	kJ/mol	Joback Method
hfus	39.42	kJ/mol	Joback Method
hvap	61.32	kJ/mol	Joback Method
log10ws	-4.07		Crippen Method
logp	3.776		Crippen Method
mcvol	228.310	ml/mol	McGowan Method
pc	1495.35	kPa	Joback Method
rinpol	1637.00		NIST Webbook
rinpol	1637.00		NIST Webbook
tb	666.88	K	Joback Method
tc	833.64	K	Joback Method
tf	396.05	K	Joback Method
vc	0.910	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	648.52	J/mol×K	666.88	Joback Method
cpg	663.04	J/mol×K	694.67	Joback Method
cpg	676.85	J/mol×K	722.47	Joback Method
cpg	689.97	J/mol×K	750.26	Joback Method
cpg	702.41	J/mol×K	778.06	Joback Method
cpg	714.19	J/mol×K	805.85	Joback Method
cpg	725.33	J/mol×K	833.64	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=U382466&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