Succinic acid, hexadecyl 2,2,2-trifluoroethyl ester

Inchi: InChI=1S/C22H39F3O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-18-28-20(26)16-17-21(27
InchiKey: ONDWRZIPRCSVOI-UHFFFAOYSA-N
Formula: C22H39F3O4
SMILES: CCCCCCCCCCCCCCCCCOC(=O)CCC(=O)OCC(F)(F)F
Mol. weight [g/mol]: 424.54

Physical Properties

Property code	Value	Unit	Source
gf	-915.07	kJ/mol	Joback Method
hf	-1584.09	kJ/mol	Joback Method
hfus	60.14	kJ/mol	Joback Method
hvap	79.13	kJ/mol	Joback Method
log10ws	-7.42		Crippen Method
logp	6.897		Crippen Method
mcvol	341.030	ml/mol	McGowan Method
pc	888.94	kPa	Joback Method
rinpol	2405.00		NIST Webbook
rinpol	2405.00		NIST Webbook
tb	849.92	K	Joback Method
tc	1041.12	K	Joback Method
tf	486.21	K	Joback Method
vc	1.359	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1114.30	J/mol×K	849.92	Joback Method
cpg	1132.90	J/mol×K	881.79	Joback Method
cpg	1150.34	J/mol×K	913.65	Joback Method
cpg	1166.65	J/mol×K	945.52	Joback Method
cpg	1181.88	J/mol×K	977.39	Joback Method
cpg	1196.06	J/mol×K	1009.26	Joback Method
cpg	1209.24	J/mol×K	1041.12	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=U382474&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