Succinic acid, pentadecyl 2,2,2-trifluoroethyl ester

Inchi: InChI=1S/C21H37F3O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-17-27-19(25)15-16-20(26)28
InchiKey: FDBNPRPOAIQYCT-UHFFFAOYSA-N
Formula: C21H37F3O4
SMILES: CCCCCCCCCCCCCCCOC(=O)CCC(=O)OCC(F)(F)F
Mol. weight [g/mol]: 410.51

Physical Properties

Property code	Value	Unit	Source
gf	-923.49	kJ/mol	Joback Method
hf	-1563.45	kJ/mol	Joback Method
hfus	57.55	kJ/mol	Joback Method
hvap	76.91	kJ/mol	Joback Method
log10ws	-7.00		Crippen Method
logp	6.507		Crippen Method
mcvol	326.940	ml/mol	McGowan Method
pc	942.10	kPa	Joback Method
rinpol	2313.00		NIST Webbook
rinpol	2313.00		NIST Webbook
tb	827.04	K	Joback Method
tc	1012.54	K	Joback Method
tf	474.94	K	Joback Method
vc	1.302	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1053.02	J/mol×K	827.04	Joback Method
cpg	1071.03	J/mol×K	857.96	Joback Method
cpg	1087.97	J/mol×K	888.87	Joback Method
cpg	1103.86	J/mol×K	919.79	Joback Method
cpg	1118.74	J/mol×K	950.70	Joback Method
cpg	1132.64	J/mol×K	981.62	Joback Method
cpg	1145.60	J/mol×K	1012.54	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=U382473&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