Succinic acid, dodecyl 2,2,2-trifluoroethyl ester

Inchi: InChI=1S/C18H31F3O4/c1-2-3-4-5-6-7-8-9-10-11-14-24-16(22)12-13-17(23)25-15-18(19
InchiKey: VBBZKOOROOBMCB-UHFFFAOYSA-N
Formula: C18H31F3O4
SMILES: CCCCCCCCCCCCOC(=O)CCC(=O)OCC(F)(F)F
Mol. weight [g/mol]: 368.43

Physical Properties

Property code	Value	Unit	Source
gf	-948.75	kJ/mol	Joback Method
hf	-1501.53	kJ/mol	Joback Method
hfus	49.78	kJ/mol	Joback Method
hvap	70.23	kJ/mol	Joback Method
log10ws	-5.74		Crippen Method
logp	5.336		Crippen Method
mcvol	284.670	ml/mol	McGowan Method
pc	1133.67	kPa	Joback Method
rinpol	2020.00		NIST Webbook
rinpol	2020.00		NIST Webbook
tb	758.40	K	Joback Method
tc	931.85	K	Joback Method
tf	441.13	K	Joback Method
vc	1.135	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	873.84	J/mol×K	758.40	Joback Method
cpg	890.30	J/mol×K	787.31	Joback Method
cpg	905.86	J/mol×K	816.22	Joback Method
cpg	920.57	J/mol×K	845.12	Joback Method
cpg	934.44	J/mol×K	874.03	Joback Method
cpg	947.49	J/mol×K	902.94	Joback Method
cpg	959.76	J/mol×K	931.85	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=U382470&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