Succinic acid, octyl 2,3,4,5-tetrafluorobenzyl ester

Inchi: InChI=1S/C19H24F4O4/c1-2-3-4-5-6-7-10-26-15(24)8-9-16(25)27-12-13-11-14(20)18(22
InchiKey: NOQJVFMTFPIKMF-UHFFFAOYSA-N
Formula: C19H24F4O4
SMILES: CCCCCCCCOC(=O)CCC(=O)OCc1cc(F)c(F)c(F)c1F
Mol. weight [g/mol]: 392.39

Physical Properties

Property code	Value	Unit	Source
gf	-1064.09	kJ/mol	Joback Method
hf	-1518.88	kJ/mol	Joback Method
hfus	55.34	kJ/mol	Joback Method
hvap	77.86	kJ/mol	Joback Method
log10ws	-6.43		Crippen Method
logp	4.970		Crippen Method
mcvol	276.770	ml/mol	McGowan Method
pc	1223.41	kPa	Joback Method
rinpol	2245.00		NIST Webbook
rinpol	2245.00		NIST Webbook
tb	830.38	K	Joback Method
tc	1019.22	K	Joback Method
tf	527.07	K	Joback Method
vc	1.111	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	846.65	J/mol×K	830.38	Joback Method
cpg	860.92	J/mol×K	861.85	Joback Method
cpg	874.21	J/mol×K	893.33	Joback Method
cpg	886.55	J/mol×K	924.80	Joback Method
cpg	897.94	J/mol×K	956.28	Joback Method
cpg	908.38	J/mol×K	987.75	Joback Method
cpg	917.88	J/mol×K	1019.22	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=U381618&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