Succinic acid, 2,2,3,3-tetrafluoropropyl 4-(4-methoxyphenyl)cyclohexyl ester

Inchi: InChI=1S/C20H24F4O5/c1-27-15-6-2-13(3-7-15)14-4-8-16(9-5-14)29-18(26)11-10-17(25

InchiKey: HHYNXCDDXQGQHR-UHFFFAOYSA-N

Formula: C20H24F4O5

SMILES: COc1ccc(C2CCC(OC(=O)CCC(=O)OCC(F)(F)C(F)F)CC2)cc1

Mol. weight [g/mol]: 420.40

Physical Properties

Property code	Value	Unit	Source
gf	-1114.64	kJ/mol	Joback Method
hf	-1617.38	kJ/mol	Joback Method
hfus	42.26	kJ/mol	Joback Method
hvap	78.94	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	4.488		Crippen Method
mcvol	285.870	ml/mol	McGowan Method
pc	1343.73	kPa	Joback Method
rinpol	2853.00		NIST Webbook
rinpol	2853.00		NIST Webbook
tb	871.95	K	Joback Method
tc	1078.69	K	Joback Method
tf	513.57	K	Joback Method
vc	1.101	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	936.42	J/mol×K	871.95	Joback Method
cpg	951.43	J/mol×K	906.41	Joback Method
cpg	965.03	J/mol×K	940.86	Joback Method
cpg	977.24	J/mol×K	975.32	Joback Method
cpg	988.08	J/mol×K	1009.78	Joback Method
cpg	997.60	J/mol×K	1044.23	Joback Method
cpg	1005.82	J/mol×K	1078.69	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=U390035&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