Succinic acid, 2,2,3,3,4,4,5,5-octafluoropentyl (2-methylcyclohex-1-en-1-yl)methyl ester

Inchi: InChI=1S/C17H20F8O4/c1-10-4-2-3-5-11(10)8-28-12(26)6-7-13(27)29-9-15(20,21)17(24

InchiKey: BSQNMOOABHSGLJ-UHFFFAOYSA-N

Formula: C17H20F8O4

SMILES: CC1=C(COC(=O)CCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F)CCCC1

Mol. weight [g/mol]: 440.33

Physical Properties

Property code	Value	Unit	Source
gf	-1885.12	kJ/mol	Joback Method
hf	-2374.72	kJ/mol	Joback Method
hfus	35.44	kJ/mol	Joback Method
hvap	63.29	kJ/mol	Joback Method
log10ws	-5.67		Crippen Method
logp	4.914		Crippen Method
mcvol	264.270	ml/mol	McGowan Method
pc	1267.35	kPa	Joback Method
rinpol	1949.00		NIST Webbook
rinpol	1949.00		NIST Webbook
tb	758.31	K	Joback Method
tc	937.54	K	Joback Method
tf	460.07	K	Joback Method
vc	1.060	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	824.10	J/mol×K	758.31	Joback Method
cpg	838.22	J/mol×K	788.18	Joback Method
cpg	851.40	J/mol×K	818.05	Joback Method
cpg	863.66	J/mol×K	847.92	Joback Method
cpg	875.08	J/mol×K	877.79	Joback Method
cpg	885.69	J/mol×K	907.67	Joback Method
cpg	895.55	J/mol×K	937.54	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=U391416&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