Succinic acid, 2,2,3,3,4,4,5,5-octafluoropentyl adamant-2-yl ester

Inchi: InChI=1S/C19H22F8O4/c20-16(21)18(24,25)19(26,27)17(22,23)8-30-13(28)1-2-14(29)31

InchiKey: FSWQMUPUKTVOEE-UHFFFAOYSA-N

Formula: C19H22F8O4

SMILES: O=C(CCC(=O)OC1C2CC3CC(C2)CC1C3)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 466.36

Physical Properties

Property code	Value	Unit	Source
gf	-1756.41	kJ/mol	Joback Method
hf	-2353.94	kJ/mol	Joback Method
hfus	43.86	kJ/mol	Joback Method
hvap	64.68	kJ/mol	Joback Method
log10ws	-5.59		Crippen Method
logp	4.849		Crippen Method
mcvol	275.030	ml/mol	McGowan Method
pc	1192.35	kPa	Joback Method
rinpol	2168.00		NIST Webbook
tb	785.88	K	Joback Method
tc	969.72	K	Joback Method
tf	487.01	K	Joback Method
vc	1.113	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	936.69	J/mol×K	785.88	Joback Method
cpg	952.63	J/mol×K	816.52	Joback Method
cpg	967.56	J/mol×K	847.16	Joback Method
cpg	981.59	J/mol×K	877.80	Joback Method
cpg	994.80	J/mol×K	908.44	Joback Method
cpg	1007.30	J/mol×K	939.08	Joback Method
cpg	1019.18	J/mol×K	969.72	Joback Method

Sources

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=U391339&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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