Succinic acid, 2,2,3,3,4,4,5,5-octafluoropentyl cyclopentyl ester

Inchi: InChI=1S/C14H16F8O4/c15-11(16)13(19,20)14(21,22)12(17,18)7-25-9(23)5-6-10(24)26-

InchiKey: BUFKNKGQZGDEDT-UHFFFAOYSA-N

Formula: C14H16F8O4

SMILES: O=C(CCC(=O)OC1CCCC1)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 400.26

Physical Properties

Property code	Value	Unit	Source
gf	-1916.69	kJ/mol	Joback Method
hf	-2361.82	kJ/mol	Joback Method
hfus	30.40	kJ/mol	Joback Method
hvap	54.52	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	3.967		Crippen Method
mcvol	226.300	ml/mol	McGowan Method
pc	1496.51	kPa	Joback Method
rinpol	1618.00		NIST Webbook
rinpol	1618.00		NIST Webbook
tb	671.61	K	Joback Method
tc	842.07	K	Joback Method
tf	399.74	K	Joback Method
vc	0.913	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	684.37	J/mol×K	671.61	Joback Method
cpg	698.59	J/mol×K	700.02	Joback Method
cpg	711.88	J/mol×K	728.43	Joback Method
cpg	724.31	J/mol×K	756.84	Joback Method
cpg	735.91	J/mol×K	785.25	Joback Method
cpg	746.72	J/mol×K	813.66	Joback Method
cpg	756.80	J/mol×K	842.07	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=U391372&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