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

Inchi: InChI=1S/C17H24F8O4/c1-10(7-14(2,3)4)8-28-11(26)5-6-12(27)29-9-15(20,21)17(24,25)

InchiKey: SKGHVJWFGRAOTQ-UHFFFAOYSA-N

Formula: C17H24F8O4

SMILES: CC(COC(=O)CCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F)CC(C)(C)C

Mol. weight [g/mol]: 444.36

Physical Properties

Property code	Value	Unit	Source
gf	-1927.58	kJ/mol	Joback Method
hf	-2498.25	kJ/mol	Joback Method
hfus	33.30	kJ/mol	Joback Method
hvap	59.25	kJ/mol	Joback Method
log10ws	-5.44		Crippen Method
logp	5.096		Crippen Method
mcvol	279.430	ml/mol	McGowan Method
pc	1092.10	kPa	Joback Method
rinpol	1681.00		NIST Webbook
rinpol	1681.00		NIST Webbook
tb	721.30	K	Joback Method
tc	888.97	K	Joback Method
tf	410.07	K	Joback Method
vc	1.123	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	861.55	J/mol×K	721.30	Joback Method
cpg	876.36	J/mol×K	749.24	Joback Method
cpg	890.27	J/mol×K	777.19	Joback Method
cpg	903.32	J/mol×K	805.13	Joback Method
cpg	915.57	J/mol×K	833.08	Joback Method
cpg	927.07	J/mol×K	861.02	Joback Method
cpg	937.87	J/mol×K	888.97	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389541&Units=SI
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

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