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

Inchi: InChI=1S/C16H22F8O4/c1-8(2)12(9(3)4)28-11(26)6-5-10(25)27-7-14(19,20)16(23,24)15

InchiKey: IBHUVQHWWCNUAQ-UHFFFAOYSA-N

Formula: C16H22F8O4

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

Mol. weight [g/mol]: 430.33

Physical Properties

Property code	Value	Unit	Source
gf	-1943.72	kJ/mol	Joback Method
hf	-2479.42	kJ/mol	Joback Method
hfus	31.08	kJ/mol	Joback Method
hvap	57.55	kJ/mol	Joback Method
log10ws	-5.13		Crippen Method
logp	4.705		Crippen Method
mcvol	265.340	ml/mol	McGowan Method
pc	1162.45	kPa	Joback Method
rinpol	1590.00		NIST Webbook
rinpol	1590.00		NIST Webbook
tb	700.77	K	Joback Method
tc	865.65	K	Joback Method
tf	366.38	K	Joback Method
vc	1.067	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	804.38	J/mol×K	700.77	Joback Method
cpg	818.96	J/mol×K	728.25	Joback Method
cpg	832.67	J/mol×K	755.73	Joback Method
cpg	845.56	J/mol×K	783.21	Joback Method
cpg	857.67	J/mol×K	810.69	Joback Method
cpg	869.04	J/mol×K	838.17	Joback Method
cpg	879.70	J/mol×K	865.65	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=U390500&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