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

Inchi: InChI=1S/C15H20F8O4/c1-8(2)6-9(3)27-11(25)5-4-10(24)26-7-13(18,19)15(22,23)14(20

InchiKey: RSLTZAOTZKTQQT-UHFFFAOYSA-N

Formula: C15H20F8O4

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

Mol. weight [g/mol]: 416.30

Physical Properties

Property code	Value	Unit	Source
gf	-1949.70	kJ/mol	Joback Method
hf	-2453.50	kJ/mol	Joback Method
hfus	32.01	kJ/mol	Joback Method
hvap	55.71	kJ/mol	Joback Method
log10ws	-4.95		Crippen Method
logp	4.459		Crippen Method
mcvol	251.250	ml/mol	McGowan Method
pc	1235.48	kPa	Joback Method
rinpol	1512.00		NIST Webbook
rinpol	1512.00		NIST Webbook
tb	678.33	K	Joback Method
tc	840.12	K	Joback Method
tf	370.11	K	Joback Method
vc	1.016	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	748.90	J/mol×K	678.33	Joback Method
cpg	762.91	J/mol×K	705.30	Joback Method
cpg	776.11	J/mol×K	732.26	Joback Method
cpg	788.54	J/mol×K	759.23	Joback Method
cpg	800.23	J/mol×K	786.19	Joback Method
cpg	811.21	J/mol×K	813.16	Joback Method
cpg	821.52	J/mol×K	840.12	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=U390422&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