Succinic acid, 2,2,3,3,4,4,5,5-octafluoropentyl hex-5-en-1-yl ester

Inchi: InChI=1S/C15H18F8O4/c1-2-3-4-5-8-26-10(24)6-7-11(25)27-9-13(18,19)15(22,23)14(20

InchiKey: XMMWPOIMXDYCMG-UHFFFAOYSA-N

Formula: C15H18F8O4

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

Mol. weight [g/mol]: 414.29

Physical Properties

Property code	Value	Unit	Source
gf	-1856.98	kJ/mol	Joback Method
hf	-2317.51	kJ/mol	Joback Method
hfus	37.77	kJ/mol	Joback Method
hvap	55.81	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	4.380		Crippen Method
mcvol	246.950	ml/mol	McGowan Method
pc	1258.37	kPa	Joback Method
rinpol	1654.00		NIST Webbook
rinpol	1654.00		NIST Webbook
tb	675.89	K	Joback Method
tc	835.97	K	Joback Method
tf	398.35	K	Joback Method
vc	1.010	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	724.57	J/mol×K	675.89	Joback Method
cpg	737.76	J/mol×K	702.57	Joback Method
cpg	750.18	J/mol×K	729.25	Joback Method
cpg	761.87	J/mol×K	755.93	Joback Method
cpg	772.87	J/mol×K	782.61	Joback Method
cpg	783.21	J/mol×K	809.29	Joback Method
cpg	792.93	J/mol×K	835.97	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=U391277&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

Latest version available from:
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