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

Inchi: InChI=1S/C11H9Cl3F8O4/c12-9(13,14)4-26-6(24)2-1-5(23)25-3-8(17,18)11(21,22)10(19

InchiKey: IJDSUOAQGAWQMZ-UHFFFAOYSA-N

Formula: C11H9Cl3F8O4

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

Mol. weight [g/mol]: 463.53

Physical Properties

Property code	Value	Unit	Source
gf	-2011.45	kJ/mol	Joback Method
hf	-2416.35	kJ/mol	Joback Method
hfus	33.87	kJ/mol	Joback Method
hvap	59.44	kJ/mol	Joback Method
log10ws	-4.97		Crippen Method
logp	4.394		Crippen Method
mcvol	231.610	ml/mol	McGowan Method
pc	1515.21	kPa	Joback Method
rinpol	1662.00		NIST Webbook
rinpol	1662.00		NIST Webbook
tb	696.75	K	Joback Method
tc	872.13	K	Joback Method
tf	447.21	K	Joback Method
vc	0.941	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	621.92	J/mol×K	696.75	Joback Method
cpg	631.23	J/mol×K	725.98	Joback Method
cpg	639.80	J/mol×K	755.21	Joback Method
cpg	647.69	J/mol×K	784.44	Joback Method
cpg	654.94	J/mol×K	813.67	Joback Method
cpg	661.61	J/mol×K	842.90	Joback Method
cpg	667.74	J/mol×K	872.13	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390228&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

Latest version available from:
https://www.chemeo.com/cid/82-819-2/Succinic-acid-2-2-3-3-4-4-5-5-octafluoropentyl-2-2-2-trichloroethyl-ester.pdf
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