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

Inchi: InChI=1S/C19H12Cl2F8O4/c20-11-7-12(21)15(10-4-2-1-3-9(10)11)33-14(31)6-5-13(30)3

InchiKey: FRDOYHNBQFVTQX-UHFFFAOYSA-N

Formula: C19H12Cl2F8O4

SMILES: O=C(CCC(=O)Oc1c(Cl)cc(Cl)c2ccccc12)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 527.19

Physical Properties

Property code	Value	Unit	Source
gf	-1744.83	kJ/mol	Joback Method
hf	-2163.79	kJ/mol	Joback Method
hfus	47.70	kJ/mol	Joback Method
hvap	80.06	kJ/mol	Joback Method
log10ws	-8.01		Crippen Method
logp	6.546		Crippen Method
mcvol	288.870	ml/mol	McGowan Method
pc	1286.51	kPa	Joback Method
rinpol	2601.00		NIST Webbook
tb	906.19	K	Joback Method
tc	1113.92	K	Joback Method
tf	601.71	K	Joback Method
vc	1.165	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	850.18	J/mol×K	906.19	Joback Method
cpg	859.62	J/mol×K	940.81	Joback Method
cpg	868.37	J/mol×K	975.43	Joback Method
cpg	876.53	J/mol×K	1010.06	Joback Method
cpg	884.20	J/mol×K	1044.68	Joback Method
cpg	891.48	J/mol×K	1079.30	Joback Method
cpg	898.46	J/mol×K	1113.92	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389901&Units=SI

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