Succinic acid, 2,2,3,3-tetrafluoropropyl 2,4-dichloronaphth-1-yl ester

Inchi: InChI=1S/C17H12Cl2F4O4/c18-11-7-12(19)15(10-4-2-1-3-9(10)11)27-14(25)6-5-13(24)2

InchiKey: ZBTSATKOUWJPFO-UHFFFAOYSA-N

Formula: C17H12Cl2F4O4

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

Mol. weight [g/mol]: 427.17

Physical Properties

Property code	Value	Unit	Source
gf	-988.11	kJ/mol	Joback Method
hf	-1320.57	kJ/mol	Joback Method
hfus	45.03	kJ/mol	Joback Method
hvap	81.47	kJ/mol	Joback Method
log10ws	-6.54		Crippen Method
logp	5.276		Crippen Method
mcvol	253.610	ml/mol	McGowan Method
pc	1660.55	kPa	Joback Method
rinpol	2530.00		NIST Webbook
rinpol	2530.00		NIST Webbook
tb	869.81	K	Joback Method
tc	1082.48	K	Joback Method
tf	571.97	K	Joback Method
vc	1.002	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	707.52	J/mol×K	869.81	Joback Method
cpg	717.37	J/mol×K	905.25	Joback Method
cpg	726.40	J/mol×K	940.70	Joback Method
cpg	734.66	J/mol×K	976.14	Joback Method
cpg	742.21	J/mol×K	1011.59	Joback Method
cpg	749.10	J/mol×K	1047.03	Joback Method
cpg	755.39	J/mol×K	1082.48	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389900&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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