Succinic acid, 2,3-dichlorophenyl 2,2,3,3-tetrafluoropropyl ester

Inchi: InChI=1S/C13H10Cl2F4O4/c14-7-2-1-3-8(11(7)15)23-10(21)5-4-9(20)22-6-13(18,19)12(1

InchiKey: OFEYFJLGBDXPBU-UHFFFAOYSA-N

Formula: C13H10Cl2F4O4

SMILES: O=C(CCC(=O)Oc1cccc(Cl)c1Cl)OCC(F)(F)C(F)F

Mol. weight [g/mol]: 377.12

Physical Properties

Property code	Value	Unit	Source
gf	-1118.81	kJ/mol	Joback Method
hf	-1417.61	kJ/mol	Joback Method
hfus	38.04	kJ/mol	Joback Method
hvap	70.26	kJ/mol	Joback Method
log10ws	-4.74		Crippen Method
logp	4.123		Crippen Method
mcvol	216.710	ml/mol	McGowan Method
pc	1890.36	kPa	Joback Method
rinpol	2024.00		NIST Webbook
rinpol	2024.00		NIST Webbook
tb	754.33	K	Joback Method
tc	953.47	K	Joback Method
tf	481.67	K	Joback Method
vc	0.857	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	569.78	J/mol×K	754.33	Joback Method
cpg	579.94	J/mol×K	787.52	Joback Method
cpg	589.32	J/mol×K	820.71	Joback Method
cpg	597.93	J/mol×K	853.90	Joback Method
cpg	605.79	J/mol×K	887.09	Joback Method
cpg	612.93	J/mol×K	920.28	Joback Method
cpg	619.37	J/mol×K	953.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390856&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