Succinic acid, 1,1,1-trifluoroprop-2-yl 2,4-dichloronaphth-1-yl ester

Inchi: InChI=1S/C17H13Cl2F3O4/c1-9(17(20,21)22)25-14(23)6-7-15(24)26-16-11-5-3-2-4-10(1

InchiKey: UNJFRBDUXLOQBS-UHFFFAOYSA-N

Formula: C17H13Cl2F3O4

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

Mol. weight [g/mol]: 409.18

Physical Properties

Property code	Value	Unit	Source
gf	-793.30	kJ/mol	Joback Method
hf	-1124.46	kJ/mol	Joback Method
hfus	41.95	kJ/mol	Joback Method
hvap	82.28	kJ/mol	Joback Method
log10ws	-6.69		Crippen Method
logp	5.326		Crippen Method
mcvol	251.840	ml/mol	McGowan Method
pc	1723.16	kPa	Joback Method
rinpol	2421.00		NIST Webbook
rinpol	2421.00		NIST Webbook
tb	870.54	K	Joback Method
tc	1088.69	K	Joback Method
tf	571.38	K	Joback Method
vc	0.985	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	700.12	J/mol×K	870.54	Joback Method
cpg	710.35	J/mol×K	906.90	Joback Method
cpg	719.71	J/mol×K	943.26	Joback Method
cpg	728.27	J/mol×K	979.62	Joback Method
cpg	736.09	J/mol×K	1015.98	Joback Method
cpg	743.22	J/mol×K	1052.33	Joback Method
cpg	749.73	J/mol×K	1088.69	Joback Method

Sources

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=U389899&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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