Succinic acid, di(2,3,4-trifluorophenyl) ester

Inchi: InChI=1S/C16H8F6O4/c17-7-1-3-9(15(21)13(7)19)25-11(23)5-6-12(24)26-10-4-2-8(18)14

InchiKey: NWBQCOPHIKHVDR-UHFFFAOYSA-N

Formula: C16H8F6O4

SMILES: O=C(CCC(=O)Oc1ccc(F)c(F)c1F)Oc1ccc(F)c(F)c1F

Mol. weight [g/mol]: 378.22

Physical Properties

Property code	Value	Unit	Source
gf	-1385.82	kJ/mol	Joback Method
hf	-1635.59	kJ/mol	Joback Method
hfus	47.00	kJ/mol	Joback Method
hvap	73.14	kJ/mol	Joback Method
log10ws	-5.74		Crippen Method
logp	3.812		Crippen Method
mcvol	214.280	ml/mol	McGowan Method
pc	1795.46	kPa	Joback Method
rinpol	2055.00		NIST Webbook
tb	796.92	K	Joback Method
tc	993.55	K	Joback Method
tf	545.90	K	Joback Method
vc	0.872	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	597.44	J/mol×K	796.92	Joback Method
cpg	607.56	J/mol×K	829.69	Joback Method
cpg	616.86	J/mol×K	862.46	Joback Method
cpg	625.34	J/mol×K	895.24	Joback Method
cpg	633.00	J/mol×K	928.01	Joback Method
cpg	639.85	J/mol×K	960.78	Joback Method
cpg	645.87	J/mol×K	993.55	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=U390774&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