Succinic acid, cyclohexylmethyl 2,3,4-trifluorophenyl ester

Inchi: InChI=1S/C17H19F3O4/c18-12-6-7-13(17(20)16(12)19)24-15(22)9-8-14(21)23-10-11-4-2

InchiKey: NNFAPFXNFYLUEV-UHFFFAOYSA-N

Formula: C17H19F3O4

SMILES: O=C(CCC(=O)Oc1ccc(F)c(F)c1F)OCC1CCCCC1

Mol. weight [g/mol]: 344.33

Physical Properties

Property code	Value	Unit	Source
gf	-852.04	kJ/mol	Joback Method
hf	-1215.70	kJ/mol	Joback Method
hfus	39.31	kJ/mol	Joback Method
hvap	73.99	kJ/mol	Joback Method
log10ws	-5.06		Crippen Method
logp	3.913		Crippen Method
mcvol	235.960	ml/mol	McGowan Method
pc	1733.22	kPa	Joback Method
rinpol	2187.00		NIST Webbook
rinpol	2187.00		NIST Webbook
tb	799.92	K	Joback Method
tc	1005.98	K	Joback Method
tf	498.80	K	Joback Method
vc	0.914	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	719.57	J/mol×K	799.92	Joback Method
cpg	734.49	J/mol×K	834.26	Joback Method
cpg	748.22	J/mol×K	868.61	Joback Method
cpg	760.79	J/mol×K	902.95	Joback Method
cpg	772.19	J/mol×K	937.29	Joback Method
cpg	782.44	J/mol×K	971.63	Joback Method
cpg	791.56	J/mol×K	1005.98	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390764&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

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