Succinic acid, cyclohexylmethyl 4-fluoro-2-methoxyphenyl ester

Inchi: InChI=1S/C18H23FO5/c1-22-16-11-14(19)7-8-15(16)24-18(21)10-9-17(20)23-12-13-5-3-

InchiKey: CKIFUJKJPFXFOT-UHFFFAOYSA-N

Formula: C18H23FO5

SMILES: COc1cc(F)ccc1OC(=O)CCC(=O)OCC1CCCCC1

Mol. weight [g/mol]: 338.37

Physical Properties

Property code	Value	Unit	Source
gf	-549.37	kJ/mol	Joback Method
hf	-964.87	kJ/mol	Joback Method
hfus	37.32	kJ/mol	Joback Method
hvap	79.60	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	3.643		Crippen Method
mcvol	252.380	ml/mol	McGowan Method
pc	1721.73	kPa	Joback Method
rinpol	2444.00		NIST Webbook
rinpol	2444.00		NIST Webbook
tb	841.70	K	Joback Method
tc	1057.51	K	Joback Method
tf	518.60	K	Joback Method
vc	0.953	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	791.10	J/mol×K	841.70	Joback Method
cpg	806.68	J/mol×K	877.67	Joback Method
cpg	820.84	J/mol×K	913.64	Joback Method
cpg	833.57	J/mol×K	949.61	Joback Method
cpg	844.90	J/mol×K	985.57	Joback Method
cpg	854.81	J/mol×K	1021.54	Joback Method
cpg	863.31	J/mol×K	1057.51	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390905&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