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

Inchi: InChI=1S/C15H17F3O5/c1-10(15(16,17)18)23-14(20)8-7-13(19)22-9-11-3-5-12(21-2)6-4

InchiKey: HNCHDMOJDHTNGL-UHFFFAOYSA-N

Formula: C15H17F3O5

SMILES: COc1ccc(COC(=O)CCC(=O)OC(C)C(F)(F)F)cc1

Mol. weight [g/mol]: 334.29

Physical Properties

Property code	Value	Unit	Source
gf	-978.67	kJ/mol	Joback Method
hf	-1352.05	kJ/mol	Joback Method
hfus	33.32	kJ/mol	Joback Method
hvap	68.51	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	3.013		Crippen Method
mcvol	224.510	ml/mol	McGowan Method
pc	1772.85	kPa	Joback Method
rinpol	1912.00		NIST Webbook
rinpol	1912.00		NIST Webbook
tb	743.40	K	Joback Method
tc	937.13	K	Joback Method
tf	453.49	K	Joback Method
vc	0.871	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	646.98	J/mol×K	743.40	Joback Method
cpg	660.30	J/mol×K	775.69	Joback Method
cpg	672.71	J/mol×K	807.98	Joback Method
cpg	684.21	J/mol×K	840.26	Joback Method
cpg	694.83	J/mol×K	872.55	Joback Method
cpg	704.57	J/mol×K	904.84	Joback Method
cpg	713.47	J/mol×K	937.13	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=U389688&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