

Succinic acid, 2,2,3,3-tetrafluoropropyl 3-methoxyphenyl ester

Inchi:	InChI=1S/C14H14F4O5/c1-21-9-3-2-4-10(7-9)23-12(20)6-5-11(19)22-8-14(17,18)13(15)
InchiKey:	VZCHSCZGZFDGTJ-UHFFFAOYSA-N
Formula:	C14H14F4O5
SMILES:	COc1cccc(OC(=O)CCC(=O)OCC(F)(F)C(F)F)c1
Mol. weight [g/mol]:	338.25

Physical Properties

Property code	Value	Unit	Source
gf	-1181.90	kJ/mol	Joback Method
hf	-1527.52	kJ/mol	Joback Method
hfus	33.81	kJ/mol	Joback Method
hvap	65.47	kJ/mol	Joback Method
log10ws	-3.49		Crippen Method
logp	2.824		Crippen Method
mcvol	212.190	ml/mol	McGowan Method
pc	1851.52	kPa	Joback Method
rinpol	1908.00		NIST Webbook
rinpol	1908.00		NIST Webbook
tb	719.79	K	Joback Method
tc	908.43	K	Joback Method
tf	442.81	K	Joback Method
vc	0.833	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.09	J/molxK	719.79	Joback Method
cpg	613.56	J/molxK	751.23	Joback Method
cpg	625.18	J/molxK	782.67	Joback Method
cpg	636.00	J/molxK	814.11	Joback Method
cpg	646.00	J/molxK	845.55	Joback Method
cpg	655.21	J/molxK	876.99	Joback Method
cpg	663.64	J/molxK	908.43	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390974&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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