

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

Inchi:	InChI=1S/C14H14F4O5/c1-21-9-4-2-3-5-10(9)23-12(20)7-6-11(19)22-8-14(17,18)13(15)
InchiKey:	OLHGJFKKSKLBKT-UHFFFAOYSA-N
Formula:	C14H14F4O5
SMILES:	COc1ccccc1OC(=O)CCC(=O)OCC(F)(F)C(F)F
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	1840.00		NIST Webbook
rinpol	1840.00		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/mol×K	719.79	Joback Method
cpg	613.56	J/mol×K	751.23	Joback Method
cpg	625.18	J/mol×K	782.67	Joback Method
cpg	636.00	J/mol×K	814.11	Joback Method
cpg	646.00	J/mol×K	845.55	Joback Method
cpg	655.21	J/mol×K	876.99	Joback Method
cpg	663.64	J/mol×K	908.43	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U389701&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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