Succinic acid, 2,2,3,3-tetrafluoropropyl 2-methoxy-5-methylphenyl ester

Inchi: InChI=1S/C15H16F4O5/c1-9-3-4-10(22-2)11(7-9)24-13(21)6-5-12(20)23-8-15(18,19)14(1

InchiKey: VCICLCVGWNUHDD-UHFFFAOYSA-N

Formula: C15H16F4O5

SMILES: COc1ccc(C)cc1OC(=O)CCC(=O)OCC(F)(F)C(F)F

Mol. weight [g/mol]: 352.28

Physical Properties

Property code	Value	Unit	Source
gf	-1183.11	kJ/mol	Joback Method
hf	-1559.63	kJ/mol	Joback Method
hfus	36.01	kJ/mol	Joback Method
hvap	68.35	kJ/mol	Joback Method
log10ws	-3.96		Crippen Method
logp	3.133		Crippen Method
mcvol	226.280	ml/mol	McGowan Method
pc	1686.56	kPa	Joback Method
rinpol	1934.00		NIST Webbook
rinpol	1934.00		NIST Webbook
tb	747.65	K	Joback Method
tc	936.60	K	Joback Method
tf	466.60	K	Joback Method
vc	0.888	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	653.76	J/mol×K	747.65	Joback Method
cpg	666.51	J/mol×K	779.14	Joback Method
cpg	678.41	J/mol×K	810.63	Joback Method
cpg	689.45	J/mol×K	842.13	Joback Method
cpg	699.66	J/mol×K	873.62	Joback Method
cpg	709.04	J/mol×K	905.11	Joback Method
cpg	717.61	J/mol×K	936.60	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=U390951&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

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