

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

Inchi:	InChI=1S/C16H18F4O5/c1-10(2)24-11-5-3-4-6-12(11)25-14(22)8-7-13(21)23-9-16(19,20
InchiKey:	VZUUVPORPVGJDN-UHFFFAOYSA-N
Formula:	C16H18F4O5
SMILES:	CC(C)Oc1ccccc1OC(=O)CCC(=O)OCC(F)(F)C(F)F
Mol. weight [g/mol]:	366.30

Physical Properties

Property code	Value	Unit	Source
gf	-1167.50	kJ/mol	Joback Method
hf	-1574.08	kJ/mol	Joback Method
hfus	35.47	kJ/mol	Joback Method
hvap	69.53	kJ/mol	Joback Method
log10ws	-4.44		Crippen Method
logp	3.603		Crippen Method
mcvol	240.370	ml/mol	McGowan Method
pc	1589.81	kPa	Joback Method
rinpol	1894.00		NIST Webbook
rinpol	1894.00		NIST Webbook
tb	765.11	K	Joback Method
tc	955.25	K	Joback Method
tf	450.35	K	Joback Method
vc	0.939	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	710.06	J/molxK	765.11	Joback Method
cpg	723.43	J/molxK	796.80	Joback Method
cpg	735.86	J/molxK	828.49	Joback Method
cpg	747.37	J/molxK	860.18	Joback Method
cpg	757.97	J/molxK	891.87	Joback Method
cpg	767.69	J/molxK	923.56	Joback Method
cpg	776.54	J/molxK	955.25	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U389784&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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