Fumaric acid, 2-isopropylphenyl 2,2,3,3-tetrafluoropropyl ester

Inchi: InChI=1S/C16H16F4O4/c1-10(2)11-5-3-4-6-12(11)24-14(22)8-7-13(21)23-9-16(19,20)15

InchiKey: CONDQYOQARIQEK-BQYQJAHWSA-N

Formula: C16H16F4O4

SMILES: CC(C)c1ccccc1OC(=O)C=CC(=O)OCC(F)(F)C(F)F

Mol. weight [g/mol]: 348.29

Physical Properties

Property code	Value	Unit	Source
gf	-982.28	kJ/mol	Joback Method
hf	-1324.64	kJ/mol	Joback Method
hfus	34.48	kJ/mol	Joback Method
hvap	67.08	kJ/mol	Joback Method
log10ws	-4.41		Crippen Method
logp	3.715		Crippen Method
mcvol	230.200	ml/mol	McGowan Method
pc	1681.03	kPa	Joback Method
rinpol	1801.00		NIST Webbook
rinpol	1801.00		NIST Webbook
tb	746.85	K	Joback Method
tc	941.95	K	Joback Method
tf	423.04	K	Joback Method
vc	0.900	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	658.30	J/mol×K	746.85	Joback Method
cpg	671.41	J/mol×K	779.37	Joback Method
cpg	683.62	J/mol×K	811.88	Joback Method
cpg	694.96	J/mol×K	844.40	Joback Method
cpg	705.48	J/mol×K	876.92	Joback Method
cpg	715.21	J/mol×K	909.44	Joback Method
cpg	724.19	J/mol×K	941.95	Joback Method

Sources

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=U405867&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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