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

Inchi: InChI=1S/C16H16F4O5/c1-10(2)24-11-5-3-4-6-12(11)25-14(22)8-7-13(21)23-9-16(19,20)15(17)18/h3-8,10,15H,9H2,1-2H3/b8-7+

InchiKey: QABJWTPPBDQQOV-BQYQJAHWSA-N

Formula: C16H16F4O5

SMILES: CC(C)Oc1ccccc1OC(=O)C=CC(=O)OCC(F)(F)C(F)F

Mol. weight [g/mol]: 364.29

Physical Properties

Property code	Value	Unit	Source
gf	-1087.28	kJ/mol	Joback Method
hf	-1456.86	kJ/mol	Joback Method
hfus	35.67	kJ/mol	Joback Method
hvap	69.49	kJ/mol	Joback Method
log10ws	-4.29		Crippen Method
logp	3.379		Crippen Method
mcvol	236.070	ml/mol	McGowan Method
pc	1657.84	kPa	Joback Method
rinpol	1866.00		NIST Webbook
rinpol	1866.00		NIST Webbook
tb	769.27	K	Joback Method
tc	964.25	K	Joback Method
tf	445.27	K	Joback Method
vc	0.918	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	685.06	J/mol×K	769.27	Joback Method
cpg	697.86	J/mol×K	801.77	Joback Method
cpg	709.73	J/mol×K	834.26	Joback Method
cpg	720.71	J/mol×K	866.76	Joback Method
cpg	730.82	J/mol×K	899.26	Joback Method
cpg	740.11	J/mol×K	931.75	Joback Method
cpg	748.58	J/mol×K	964.25	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=U405707&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