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

Inchi: InChI=1S/C14H12F4O5/c1-21-9-4-2-3-5-10(9)23-12(20)7-6-11(19)22-8-14(17,18)13(15)1

InchiKey: KUSMZDGVRCWESS-VOTSOKGWSA-N

Formula: C14H12F4O5

SMILES: COc1ccccc1OC(=O)C=CC(=O)OCC(F)(F)C(F)F

Mol. weight [g/mol]: 336.24

Physical Properties

Property code	Value	Unit	Source
gf	-1101.68	kJ/mol	Joback Method
hf	-1410.30	kJ/mol	Joback Method
hfus	34.02	kJ/mol	Joback Method
hvap	65.42	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	2.600		Crippen Method
mcvol	207.890	ml/mol	McGowan Method
pc	1937.24	kPa	Joback Method
rinpol	1823.00		NIST Webbook
rinpol	1823.00		NIST Webbook
tb	723.95	K	Joback Method
tc	918.20	K	Joback Method
tf	437.73	K	Joback Method
vc	0.812	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	577.15	J/mol×K	723.95	Joback Method
cpg	589.01	J/mol×K	756.32	Joback Method
cpg	600.04	J/mol×K	788.70	Joback Method
cpg	610.26	J/mol×K	821.07	Joback Method
cpg	619.70	J/mol×K	853.45	Joback Method
cpg	628.38	J/mol×K	885.82	Joback Method
cpg	636.33	J/mol×K	918.20	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405926&Units=SI
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

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