2-Methoxybenzoic acid, 2,3,4,5-tetrafluorobenzyl ester

Inchi: InChI=1S/C15H10F4O3/c1-21-11-5-3-2-4-9(11)15(20)22-7-8-6-10(16)13(18)14(19)12(8)1

InchiKey: RTELUQNVDVBLLI-UHFFFAOYSA-N

Formula: C15H10F4O3

SMILES: COc1ccccc1C(=O)OCc1cc(F)c(F)c(F)c1F

Mol. weight [g/mol]: 314.23

Physical Properties

Property code	Value	Unit	Source
gf	-866.07	kJ/mol	Joback Method
hf	-1098.68	kJ/mol	Joback Method
hfus	37.04	kJ/mol	Joback Method
hvap	65.14	kJ/mol	Joback Method
log10ws	-5.27		Crippen Method
logp	3.609		Crippen Method
mcvol	195.080	ml/mol	McGowan Method
pc	2025.41	kPa	Joback Method
rinpol	1905.00		NIST Webbook
rinpol	1905.00		NIST Webbook
tb	716.65	K	Joback Method
tc	919.03	K	Joback Method
tf	471.00	K	Joback Method
vc	0.773	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	518.78	J/mol×K	716.65	Joback Method
cpg	530.83	J/mol×K	750.38	Joback Method
cpg	542.09	J/mol×K	784.11	Joback Method
cpg	552.55	J/mol×K	817.84	Joback Method
cpg	562.21	J/mol×K	851.57	Joback Method
cpg	571.07	J/mol×K	885.30	Joback Method
cpg	579.14	J/mol×K	919.03	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=U374923&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