Benzoic acid, (2,3,4,5-tetrafluorophenyl)methyl ester

Inchi: InChI=1S/C14H8F4O2/c15-10-6-9(11(16)13(18)12(10)17)7-20-14(19)8-4-2-1-3-5-8/h1-6H

InchiKey: QSTMIULCOVQQIB-UHFFFAOYSA-N

Formula: C14H8F4O2

SMILES: O=C(OCc1cc(F)c(F)c(F)c1F)c1ccccc1

Mol. weight [g/mol]: 284.21

Physical Properties

Property code	Value	Unit	Source
gf	-759.86	kJ/mol	Joback Method
hf	-934.35	kJ/mol	Joback Method
hfus	33.65	kJ/mol	Joback Method
hvap	59.85	kJ/mol	Joback Method
log10ws	-5.15		Crippen Method
logp	3.600		Crippen Method
mcvol	175.120	ml/mol	McGowan Method
pc	2280.59	kPa	Joback Method
rinpol	1720.00		NIST Webbook
rinpol	1720.00		NIST Webbook
tb	666.37	K	Joback Method
tc	872.00	K	Joback Method
tf	424.98	K	Joback Method
vc	0.700	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	444.06	J/mol×K	666.37	Joback Method
cpg	455.91	J/mol×K	700.64	Joback Method
cpg	466.99	J/mol×K	734.91	Joback Method
cpg	477.31	J/mol×K	769.19	Joback Method
cpg	486.89	J/mol×K	803.46	Joback Method
cpg	495.73	J/mol×K	837.73	Joback Method
cpg	503.86	J/mol×K	872.00	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=U368908&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