Benzoic acid, 3,4,5-trifluorophenylmethyl ester

Inchi: InChI=1S/C14H9F3O2/c15-11-6-9(7-12(16)13(11)17)8-19-14(18)10-4-2-1-3-5-10/h1-7H,8
InchiKey: DMNPFTSXGQXEBJ-UHFFFAOYSA-N
Formula: C14H9F3O2
SMILES: O=C(OCc1cc(F)c(F)c(F)c1)c1ccccc1
Mol. weight [g/mol]: 266.22

Physical Properties

Property code	Value	Unit	Source
gf	-555.42	kJ/mol	Joback Method
hf	-726.77	kJ/mol	Joback Method
hfus	30.96	kJ/mol	Joback Method
hvap	60.00	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	3.461		Crippen Method
mcvol	173.350	ml/mol	McGowan Method
pc	2417.12	kPa	Joback Method
rinpol	1762.00		NIST Webbook
rinpol	1762.00		NIST Webbook
tb	662.12	K	Joback Method
tc	875.83	K	Joback Method
tf	411.87	K	Joback Method
vc	0.681	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	437.13	J/mol×K	662.12	Joback Method
cpg	449.73	J/mol×K	697.74	Joback Method
cpg	461.47	J/mol×K	733.36	Joback Method
cpg	472.37	J/mol×K	768.97	Joback Method
cpg	482.45	J/mol×K	804.59	Joback Method
cpg	491.73	J/mol×K	840.21	Joback Method
cpg	500.23	J/mol×K	875.83	Joback Method

Sources

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=U367920&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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