Benzoic acid, (3-fluorophenyl)methyl ester

Inchi: InChI=1S/C14H11FO2/c15-13-8-4-5-11(9-13)10-17-14(16)12-6-2-1-3-7-12/h1-9H,10H2
InchiKey: SOXMVJFDVWBBTL-UHFFFAOYSA-N
Formula: C14H11FO2
SMILES: O=C(OCc1cccc(F)c1)c1ccccc1
Mol. weight [g/mol]: 230.23

Physical Properties

Property code	Value	Unit	Source
gf	-146.54	kJ/mol	Joback Method
hf	-311.61	kJ/mol	Joback Method
hfus	25.58	kJ/mol	Joback Method
hvap	60.31	kJ/mol	Joback Method
log10ws	-4.16		Crippen Method
logp	3.183		Crippen Method
mcvol	169.810	ml/mol	McGowan Method
pc	2729.71	kPa	Joback Method
rinpol	1786.00		NIST Webbook
rinpol	1786.00		NIST Webbook
tb	653.62	K	Joback Method
tc	885.85	K	Joback Method
tf	385.65	K	Joback Method
vc	0.645	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	423.07	J/mol×K	653.62	Joback Method
cpg	437.41	J/mol×K	692.32	Joback Method
cpg	450.65	J/mol×K	731.03	Joback Method
cpg	462.85	J/mol×K	769.73	Joback Method
cpg	474.04	J/mol×K	808.44	Joback Method
cpg	484.27	J/mol×K	847.14	Joback Method
cpg	493.58	J/mol×K	885.85	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=U368723&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