Pentafluorobenzoic acid, 3-ethylphenyl ester

Other names: 3-Ethylphenol, pentafluorobenzoyl ester
Inchi: InChI=1S/C15H9F5O2/c1-2-7-4-3-5-8(6-7)22-15(21)9-10(16)12(18)14(20)13(19)11(9)17/
InchiKey: QKQHDUIRUAMJNN-UHFFFAOYSA-N
Formula: C15H9F5O2
SMILES: CCc1cccc(OC(=O)c2c(F)c(F)c(F)c(F)c2F)c1
Mol. weight [g/mol]: 316.22

Physical Properties

Property code	Value	Unit	Source
gf	-965.51	kJ/mol	Joback Method
hf	-1174.04	kJ/mol	Joback Method
hfus	38.54	kJ/mol	Joback Method
hvap	62.58	kJ/mol	Joback Method
log10ws	-6.02		Crippen Method
logp	4.164		Crippen Method
mcvol	190.980	ml/mol	McGowan Method
pc	1949.23	kPa	Joback Method
rinpol	1679.00		NIST Webbook
rinpol	1669.30		NIST Webbook
rinpol	1671.70		NIST Webbook
rinpol	1670.20		NIST Webbook
rinpol	1669.30		NIST Webbook
tb	698.48	K	Joback Method
tc	895.55	K	Joback Method
tf	461.88	K	Joback Method
vc	0.773	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	500.33	J/mol×K	698.48	Joback Method
cpg	511.95	J/mol×K	731.33	Joback Method
cpg	522.86	J/mol×K	764.17	Joback Method
cpg	533.06	J/mol×K	797.02	Joback Method

cpg	542.56	J/mol×K	829.86	Joback Method
cpg	551.36	J/mol×K	862.71	Joback Method
cpg	559.47	J/mol×K	895.55	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360628&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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