3-Ethylphenol, O-heptafluorobutyryl-

Inchi: InChI=1S/C12H9F7O2/c1-2-7-4-3-5-8(6-7)21-9(20)10(13,14)11(15,16)12(17,18)19/h3-6H
InchiKey: GQMIHPWXWPVYRJ-UHFFFAOYSA-N
Formula: C12H9F7O2
SMILES: CCc1cccc(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)c1
Mol. weight [g/mol]: 318.19

Physical Properties

Property code	Value	Unit	Source
gf	-1436.13	kJ/mol	Joback Method
hf	-1709.77	kJ/mol	Joback Method
hfus	22.59	kJ/mol	Joback Method
hvap	44.79	kJ/mol	Joback Method
log10ws	-4.72		Crippen Method
logp	3.987		Crippen Method
mcvol	176.010	ml/mol	McGowan Method
pc	1947.51	kPa	Joback Method
rinpol	1115.00		NIST Webbook
rinpol	1115.00		NIST Webbook
tb	567.11	K	Joback Method
tc	744.88	K	Joback Method
tf	347.49	K	Joback Method
vc	0.717	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	461.01	J/mol×K	567.11	Joback Method
cpg	473.74	J/mol×K	596.74	Joback Method
cpg	485.57	J/mol×K	626.37	Joback Method
cpg	496.55	J/mol×K	655.99	Joback Method
cpg	506.73	J/mol×K	685.62	Joback Method
cpg	516.15	J/mol×K	715.25	Joback Method
cpg	524.87	J/mol×K	744.88	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=U374275&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