2,4-Difluorobenzoic acid, 3-ethylphenyl ester

Inchi: InChI=1S/C15H12F2O2/c1-2-10-4-3-5-12(8-10)19-15(18)13-7-6-11(16)9-14(13)17/h3-9H
InchiKey: WTPBFFIUTFWTNU-UHFFFAOYSA-N
Formula: C15H12F2O2
SMILES: CCc1cccc(OC(=O)c2ccc(F)cc2F)c1
Mol. weight [g/mol]: 262.25

Physical Properties

Property code	Value	Unit	Source
gf	-352.19	kJ/mol	Joback Method
hf	-551.30	kJ/mol	Joback Method
hfus	30.47	kJ/mol	Joback Method
hvap	63.04	kJ/mol	Joback Method
log10ws	-5.02		Crippen Method
logp	3.746		Crippen Method
mcvol	185.670	ml/mol	McGowan Method
pc	2300.32	kPa	Joback Method
rinpol	1842.00		NIST Webbook
rinpol	1842.00		NIST Webbook
tb	685.73	K	Joback Method
tc	905.30	K	Joback Method
tf	422.55	K	Joback Method
vc	0.720	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	479.81	J/mol×K	685.73	Joback Method
cpg	493.59	J/mol×K	722.32	Joback Method
cpg	506.40	J/mol×K	758.92	Joback Method
cpg	518.28	J/mol×K	795.51	Joback Method
cpg	529.25	J/mol×K	832.11	Joback Method
cpg	539.34	J/mol×K	868.70	Joback Method
cpg	548.57	J/mol×K	905.30	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360560&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

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