2,5-Difluorobenzoic acid, 2-ethylhexyl ester

Inchi: InChI=1S/C15H20F2O2/c1-3-5-6-11(4-2)10-19-15(18)13-9-12(16)7-8-14(13)17/h7-9,11H
InchiKey: WTUIPCHOXRRUJE-UHFFFAOYSA-N
Formula: C15H20F2O2
SMILES: CCCCC(CC)COC(=O)c1cc(F)ccc1F
Mol. weight [g/mol]: 270.31

Physical Properties

Property code	Value	Unit	Source
gf	-457.41	kJ/mol	Joback Method
hf	-781.64	kJ/mol	Joback Method
hfus	33.29	kJ/mol	Joback Method
hvap	59.72	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	4.338		Crippen Method
mcvol	209.430	ml/mol	McGowan Method
pc	1746.28	kPa	Joback Method
rinpol	1704.00		NIST Webbook
rinpol	1704.00		NIST Webbook
tb	653.63	K	Joback Method
tc	840.96	K	Joback Method
tf	368.61	K	Joback Method
vc	0.822	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	562.18	J/mol×K	653.63	Joback Method
cpg	577.57	J/mol×K	684.85	Joback Method
cpg	592.15	J/mol×K	716.07	Joback Method
cpg	605.95	J/mol×K	747.29	Joback Method
cpg	618.98	J/mol×K	778.51	Joback Method
cpg	631.26	J/mol×K	809.74	Joback Method
cpg	642.80	J/mol×K	840.96	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=U357577&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

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