

2-Ethylbutyric acid, 2-fluorophenyl ester

Inchi:	InChI=1S/C12H15FO2/c1-3-9(4-2)12(14)15-11-8-6-5-7-10(11)13/h5-9H,3-4H2,1-2H3
InchiKey:	QOUDMYRCBHVRPK-UHFFFAOYSA-N
Formula:	C12H15FO2
SMILES:	CCC(CC)C(=O)Oc1ccccc1F
Mol. weight [g/mol]:	210.24

Physical Properties

Property code	Value	Unit	Source
gf	-278.23	kJ/mol	Joback Method
hf	-512.14	kJ/mol	Joback Method
hfus	22.83	kJ/mol	Joback Method
hvap	53.20	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	3.167		Crippen Method
mcvol	165.390	ml/mol	McGowan Method
pc	2391.19	kPa	Joback Method
rinpol	1364.00		NIST Webbook
tb	580.74	K	Joback Method
tc	782.26	K	Joback Method
tf	321.69	K	Joback Method
vc	0.635	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	402.33	J/mol×K	580.74	Joback Method
cpg	416.88	J/mol×K	614.33	Joback Method
cpg	430.65	J/mol×K	647.91	Joback Method
cpg	443.66	J/mol×K	681.50	Joback Method
cpg	455.91	J/mol×K	715.09	Joback Method
cpg	467.43	J/mol×K	748.67	Joback Method
cpg	478.23	J/mol×K	782.26	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=U370145&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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