4-Fluorobenzoic acid, 3-methylbutyl ester

Inchi: InChI=1S/C12H15FO2/c1-9(2)7-8-15-12(14)10-3-5-11(13)6-4-10/h3-6,9H,7-8H2,1-2H3
InchiKey: UYMZAHGVRJBELF-UHFFFAOYSA-N
Formula: C12H15FO2
SMILES: CC(C)CCOC(=O)c1ccc(F)cc1
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	-3.48		Crippen Method
logp	3.029		Crippen Method
mcvol	165.390	ml/mol	McGowan Method
pc	2391.19	kPa	Joback Method
rinpol	1451.00		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:	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=U355673&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