3,4-Difluorobenzoic acid, isobutyl ester

Inchi: InChI=1S/C11H12F2O2/c1-7(2)6-15-11(14)8-3-4-9(12)10(13)5-8/h3-5,7H,6H2,1-2H3
InchiKey: PPYCLYDJFPQOKQ-UHFFFAOYSA-N
Formula: C11H12F2O2
SMILES: CC(C)COC(=O)c1ccc(F)c(F)c1
Mol. weight [g/mol]: 214.21

Physical Properties

Property code	Value	Unit	Source
gf	-491.09	kJ/mol	Joback Method
hf	-699.08	kJ/mol	Joback Method
hfus	22.93	kJ/mol	Joback Method
hvap	50.81	kJ/mol	Joback Method
log10ws	-3.39		Crippen Method
logp	2.778		Crippen Method
mcvol	153.070	ml/mol	McGowan Method
pc	2477.65	kPa	Joback Method
rinpol	1279.00		NIST Webbook
rinpol	1279.00		NIST Webbook
tb	562.11	K	Joback Method
tc	758.12	K	Joback Method
tf	323.53	K	Joback Method
vc	0.598	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	362.64	J/mol×K	562.11	Joback Method
cpg	375.53	J/mol×K	594.78	Joback Method
cpg	387.76	J/mol×K	627.45	Joback Method
cpg	399.36	J/mol×K	660.11	Joback Method
cpg	410.33	J/mol×K	692.78	Joback Method
cpg	420.69	J/mol×K	725.45	Joback Method
cpg	430.43	J/mol×K	758.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U338859&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

Latest version available from:
https://www.chemeo.com/cid/113-307-5/3-4-Difluorobenzoic-acid-isobutyl-ester.pdf
Generated by Cheméo on 2024-04-20 12:17:48.428208401 +0000 UTC m=+15904717.348785714.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.