2,6-Difluoro-3-methylbenzoic acid, 2-methylbutyl ester

Inchi: InChI=1S/C13H16F2O2/c1-4-8(2)7-17-13(16)11-10(14)6-5-9(3)12(11)15/h5-6,8H,4,7H2,1

InchiKey: GECDLUFFSQWEFF-UHFFFAOYSA-N

Formula: C13H16F2O2

SMILES: CCC(C)COC(=O)c1c(F)ccc(C)c1F

Mol. weight [g/mol]: 242.26

Physical Properties

Property code	Value	Unit	Source
gf	-483.88	kJ/mol	Joback Method
hf	-751.83	kJ/mol	Joback Method
hfus	27.72	kJ/mol	Joback Method
hvap	55.93	kJ/mol	Joback Method
log10ws	-4.29		Crippen Method
logp	3.476		Crippen Method
mcvol	181.250	ml/mol	McGowan Method
pc	2036.39	kPa	Joback Method
rinpol	1558.00		NIST Webbook
rinpol	1558.00		NIST Webbook
tb	612.85	K	Joback Method
tc	804.91	K	Joback Method
tf	358.59	K	Joback Method
vc	0.710	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	458.91	J/mol×K	612.85	Joback Method
cpg	473.01	J/mol×K	644.86	Joback Method
cpg	486.42	J/mol×K	676.87	Joback Method
cpg	499.14	J/mol×K	708.88	Joback Method
cpg	511.18	J/mol×K	740.89	Joback Method
cpg	522.54	J/mol×K	772.90	Joback Method
cpg	533.24	J/mol×K	804.91	Joback Method

Sources

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=U343750&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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/120-601-0/2-6-Difluoro-3-methylbenzoic-acid-2-methylbutyl-ester.pdf
Generated by Cheméo on 2024-05-20 13:42:55.357315241 +0000 UTC m=+18501824.277892563.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.