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

Inchi: InChI=1S/C12H14F2O2/c1-3-4-7-16-12(15)10-9(13)6-5-8(2)11(10)14/h5-6H,3-4,7H2,1-2
InchiKey: YDVFVNORRRMMNQ-UHFFFAOYSA-N
Formula: C12H14F2O2
SMILES: CCCCOC(=O)c1c(F)ccc(C)c1F
Mol. weight [g/mol]: 228.24

Physical Properties

Property code	Value	Unit	Source
gf	-489.86	kJ/mol	Joback Method
hf	-725.91	kJ/mol	Joback Method
hfus	28.66	kJ/mol	Joback Method
hvap	54.09	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	3.230		Crippen Method
mcvol	167.160	ml/mol	McGowan Method
pc	2208.29	kPa	Joback Method
rinpol	1496.00		NIST Webbook
rinpol	1496.00		NIST Webbook
tb	590.41	K	Joback Method
tc	781.18	K	Joback Method
tf	362.32	K	Joback Method
vc	0.659	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.34	J/mol×K	590.41	Joback Method
cpg	422.45	J/mol×K	622.20	Joback Method
cpg	434.95	J/mol×K	654.00	Joback Method
cpg	446.83	J/mol×K	685.79	Joback Method
cpg	458.10	J/mol×K	717.59	Joback Method
cpg	468.77	J/mol×K	749.38	Joback Method
cpg	478.84	J/mol×K	781.18	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U338840&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

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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