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

Inchi: InChI=1S/C11H12F2O3/c1-7-3-4-8(12)9(10(7)13)11(14)16-6-5-15-2/h3-4H,5-6H2,1-2H3

InchiKey: HLFABNDBTMQQHB-UHFFFAOYSA-N

Formula: C11H12F2O3

SMILES: COCCOC(=O)c1c(F)ccc(C)c1F

Mol. weight [g/mol]: 230.21

Physical Properties

Property code	Value	Unit	Source
gf	-603.28	kJ/mol	Joback Method
hf	-837.49	kJ/mol	Joback Method
hfus	27.25	kJ/mol	Joback Method
hvap	54.27	kJ/mol	Joback Method
log10ws	-2.78		Crippen Method
logp	2.076		Crippen Method
mcvol	158.940	ml/mol	McGowan Method
pc	2381.86	kPa	Joback Method
rinpol	1522.00		NIST Webbook
rinpol	1522.00		NIST Webbook
tb	589.95	K	Joback Method
tc	781.64	K	Joback Method
tf	373.28	K	Joback Method
vc	0.622	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	386.09	J/mol×K	589.95	Joback Method
cpg	398.28	J/mol×K	621.90	Joback Method
cpg	409.93	J/mol×K	653.85	Joback Method
cpg	421.02	J/mol×K	685.80	Joback Method
cpg	431.56	J/mol×K	717.75	Joback Method
cpg	441.54	J/mol×K	749.69	Joback Method
cpg	450.94	J/mol×K	781.64	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=U343749&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