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

Inchi: InChI=1S/C12H14F2O3/c1-3-16-6-7-17-12(15)10-9(13)5-4-8(2)11(10)14/h4-5H,3,6-7H2,
InchiKey: JKLGZVWNLXTWJO-UHFFFAOYSA-N
Formula: C12H14F2O3
SMILES: CCOCCOC(=O)c1c(F)ccc(C)c1F
Mol. weight [g/mol]: 244.23

Physical Properties

Property code	Value	Unit	Source
gf	-594.86	kJ/mol	Joback Method
hf	-858.13	kJ/mol	Joback Method
hfus	29.85	kJ/mol	Joback Method
hvap	56.50	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	2.467		Crippen Method
mcvol	173.030	ml/mol	McGowan Method
pc	2173.43	kPa	Joback Method
rinpol	1580.00		NIST Webbook
rinpol	1580.00		NIST Webbook
tb	612.83	K	Joback Method
tc	802.33	K	Joback Method
tf	384.55	K	Joback Method
vc	0.677	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	434.50	J/mol×K	612.83	Joback Method
cpg	447.45	J/mol×K	644.41	Joback Method
cpg	459.81	J/mol×K	676.00	Joback Method
cpg	471.56	J/mol×K	707.58	Joback Method
cpg	482.71	J/mol×K	739.16	Joback Method
cpg	493.24	J/mol×K	770.75	Joback Method
cpg	503.16	J/mol×K	802.33	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U343751&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