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

Inchi: InChI=1S/C12H15F2NO2/c1-8-4-5-9(13)10(11(8)14)12(16)17-7-6-15(2)3/h4-5H,6-7H2,1-

InchiKey: HUWOLAOZCUQHAP-UHFFFAOYSA-N

Formula: C12H15F2NO2

SMILES: Cc1ccc(F)c(C(=O)OCCN(C)C)c1F

Mol. weight [g/mol]: 243.25

Physical Properties

Property code	Value	Unit	Source
gf	-379.08	kJ/mol	Joback Method
hf	-658.38	kJ/mol	Joback Method
hfus	31.68	kJ/mol	Joback Method
hvap	56.13	kJ/mol	Joback Method
log10ws	-2.68		Crippen Method
logp	1.992		Crippen Method
mcvol	177.140	ml/mol	McGowan Method
pc	2204.15	kPa	Joback Method
rinpol	1622.00		NIST Webbook
rinpol	1622.00		NIST Webbook
tb	602.85	K	Joback Method
tc	791.53	K	Joback Method
tf	394.79	K	Joback Method
vc	0.677	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.83	J/mol×K	602.85	Joback Method
cpg	459.43	J/mol×K	634.30	Joback Method
cpg	472.35	J/mol×K	665.74	Joback Method
cpg	484.59	J/mol×K	697.19	Joback Method
cpg	496.17	J/mol×K	728.64	Joback Method
cpg	507.10	J/mol×K	760.08	Joback Method
cpg	517.39	J/mol×K	791.53	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U343752&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