6-Fluoro-3-trifluoromethylbenzoic acid, 2-dimethylaminoethyl ester

Other names: 6-Fluoro-3-trifluorobenzoic acid, 2-dimethylaminoethyl ester
Inchi: InChI=1S/C12H13F4NO2/c1-17(2)5-6-19-11(18)9-7-8(12(14,15)16)3-4-10(9)13/h3-4,7H,
InchiKey: SLOQOUDOFJEKOQ-UHFFFAOYSA-N
Formula: C12H13F4NO2
SMILES: CN(C)CCOC(=O)c1cc(C(F)(F)F)ccc1F
Mol. weight [g/mol]: 279.23

Physical Properties

Property code	Value	Unit	Source
gf	-756.23	kJ/mol	Joback Method
hf	-1047.88	kJ/mol	Joback Method
hfus	30.81	kJ/mol	Joback Method
hvap	52.54	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	2.563		Crippen Method
mcvol	180.680	ml/mol	McGowan Method
pc	2092.66	kPa	Joback Method
rinpol	1488.00		NIST Webbook
rinpol	1488.00		NIST Webbook
tb	593.18	K	Joback Method
tc	774.75	K	Joback Method
tf	385.87	K	Joback Method
vc	0.703	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	465.78	J/mol×K	593.18	Joback Method
cpg	479.04	J/mol×K	623.44	Joback Method
cpg	491.53	J/mol×K	653.70	Joback Method
cpg	503.28	J/mol×K	683.97	Joback Method
cpg	514.32	J/mol×K	714.23	Joback Method
cpg	524.68	J/mol×K	744.49	Joback Method
cpg	534.39	J/mol×K	774.75	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U343782&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