2,5-Di(trifluoromethyl)benzoic acid, 2-(dimethylamino)ethyl ester

Inchi: InChI=1S/C13H13F6NO2/c1-20(2)5-6-22-11(21)9-7-8(12(14,15)16)3-4-10(9)13(17,18)19

InchiKey: QSHYNHMMXCRJID-UHFFFAOYSA-N

Formula: C13H13F6NO2

SMILES: CN(C)CCOC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F

Mol. weight [g/mol]: 329.24

Physical Properties

Property code	Value	Unit	Source
gf	-1134.59	kJ/mol	Joback Method
hf	-1469.49	kJ/mol	Joback Method
hfus	32.15	kJ/mol	Joback Method
hvap	51.84	kJ/mol	Joback Method
log10ws	-3.75		Crippen Method
logp	3.443		Crippen Method
mcvol	198.310	ml/mol	McGowan Method
pc	1806.16	kPa	Joback Method
rinpol	1420.00		NIST Webbook
tb	611.37	K	Joback Method
tc	785.94	K	Joback Method
tf	400.74	K	Joback Method
vc	0.783	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	534.97	J/mol×K	611.37	Joback Method
cpg	548.20	J/mol×K	640.47	Joback Method
cpg	560.62	J/mol×K	669.56	Joback Method
cpg	572.25	J/mol×K	698.66	Joback Method
cpg	583.14	J/mol×K	727.75	Joback Method
cpg	593.32	J/mol×K	756.85	Joback Method
cpg	602.84	J/mol×K	785.94	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357365&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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