2,5-Di(trifluoromethyl)benzoic acid, 2-methoxyethyl ester

Inchi: InChI=1S/C12H10F6O3/c1-20-4-5-21-10(19)8-6-7(11(13,14)15)2-3-9(8)12(16,17)18/h2-3

InchiKey: IPNKALWCIHQLKD-UHFFFAOYSA-N

Formula: C12H10F6O3

SMILES: COCCOC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F

Mol. weight [g/mol]: 316.20

Physical Properties

Property code	Value	Unit	Source
gf	-1358.79	kJ/mol	Joback Method
hf	-1648.60	kJ/mol	Joback Method
hfus	27.73	kJ/mol	Joback Method
hvap	49.98	kJ/mol	Joback Method
log10ws	-3.85		Crippen Method
logp	3.527		Crippen Method
mcvol	180.110	ml/mol	McGowan Method
pc	1937.24	kPa	Joback Method
rinpol	1286.00		NIST Webbook
tb	598.47	K	Joback Method
tc	775.15	K	Joback Method
tf	379.23	K	Joback Method
vc	0.728	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	474.34	J/mol×K	598.47	Joback Method
cpg	486.39	J/mol×K	627.92	Joback Method
cpg	497.72	J/mol×K	657.36	Joback Method
cpg	508.35	J/mol×K	686.81	Joback Method
cpg	518.32	J/mol×K	716.25	Joback Method
cpg	527.65	J/mol×K	745.70	Joback Method
cpg	536.35	J/mol×K	775.15	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357361&Units=SI

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