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

Inchi: InChI=1S/C11H7ClF6O2/c12-3-4-20-9(19)7-5-6(10(13,14)15)1-2-8(7)11(16,17)18/h1-2,5

InchiKey: NNBVMAMVBRTAKV-UHFFFAOYSA-N

Formula: C11H7ClF6O2

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

Mol. weight [g/mol]: 320.62

Physical Properties

Property code	Value	Unit	Source
gf	-1274.14	kJ/mol	Joback Method
hf	-1511.48	kJ/mol	Joback Method
hfus	28.14	kJ/mol	Joback Method
hvap	49.73	kJ/mol	Joback Method
log10ws	-4.49		Crippen Method
logp	4.120		Crippen Method
mcvol	172.390	ml/mol	McGowan Method
pc	2073.65	kPa	Joback Method
rinpol	1306.00		NIST Webbook
tb	590.60	K	Joback Method
tc	774.02	K	Joback Method
tf	375.65	K	Joback Method
vc	0.703	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	428.35	J/mol×K	590.60	Joback Method
cpg	439.18	J/mol×K	621.17	Joback Method
cpg	449.26	J/mol×K	651.74	Joback Method
cpg	458.64	J/mol×K	682.31	Joback Method
cpg	467.35	J/mol×K	712.88	Joback Method
cpg	475.42	J/mol×K	743.45	Joback Method
cpg	482.90	J/mol×K	774.02	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357362&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