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

Inchi: InChI=1S/C12H10F6O2/c1-2-5-20-10(19)8-6-7(11(13,14)15)3-4-9(8)12(16,17)18/h3-4,6H

InchiKey: ORFWPYIFRFMVHX-UHFFFAOYSA-N

Formula: C12H10F6O2

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

Mol. weight [g/mol]: 300.20

Physical Properties

Property code	Value	Unit	Source
gf	-1253.79	kJ/mol	Joback Method
hf	-1516.38	kJ/mol	Joback Method
hfus	26.54	kJ/mol	Joback Method
hvap	47.57	kJ/mol	Joback Method
log10ws	-4.76		Crippen Method
logp	4.291		Crippen Method
mcvol	174.240	ml/mol	McGowan Method
pc	1966.56	kPa	Joback Method
rinpol	1200.00		NIST Webbook
rinpol	1200.00		NIST Webbook
tb	576.05	K	Joback Method
tc	753.32	K	Joback Method
tf	357.00	K	Joback Method
vc	0.710	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	449.21	J/mol×K	576.05	Joback Method
cpg	461.56	J/mol×K	605.59	Joback Method
cpg	473.13	J/mol×K	635.14	Joback Method
cpg	483.98	J/mol×K	664.68	Joback Method
cpg	494.14	J/mol×K	694.23	Joback Method
cpg	503.63	J/mol×K	723.77	Joback Method
cpg	512.50	J/mol×K	753.32	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=U338934&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