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

Inchi: InChI=1S/C13H12F6O2/c1-7(2)6-21-11(20)9-5-8(12(14,15)16)3-4-10(9)13(17,18)19/h3-5

InchiKey: FIGJSQCQCQNPTL-UHFFFAOYSA-N

Formula: C13H12F6O2

SMILES: CC(C)COC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F

Mol. weight [g/mol]: 314.22

Physical Properties

Property code	Value	Unit	Source
gf	-1247.81	kJ/mol	Joback Method
hf	-1542.30	kJ/mol	Joback Method
hfus	25.61	kJ/mol	Joback Method
hvap	49.41	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	4.537		Crippen Method
mcvol	188.330	ml/mol	McGowan Method
pc	1821.61	kPa	Joback Method
rinpol	1233.00		NIST Webbook
rinpol	1233.00		NIST Webbook
tb	598.49	K	Joback Method
tc	777.41	K	Joback Method
tf	353.27	K	Joback Method
vc	0.759	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	498.28	J/mol×K	598.49	Joback Method
cpg	511.43	J/mol×K	628.31	Joback Method
cpg	523.77	J/mol×K	658.13	Joback Method
cpg	535.33	J/mol×K	687.95	Joback Method
cpg	546.14	J/mol×K	717.77	Joback Method
cpg	556.26	J/mol×K	747.59	Joback Method
cpg	565.70	J/mol×K	777.41	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=U338935&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