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

Inchi: InChI=1S/C14H14F6O2/c1-3-8(2)7-22-12(21)10-6-9(13(15,16)17)4-5-11(10)14(18,19)20/
InchiKey: MEWZYRLJFCRUKX-UHFFFAOYSA-N
Formula: C14H14F6O2
SMILES: CCC(C)COC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F
Mol. weight [g/mol]: 328.25

Physical Properties

Property code	Value	Unit	Source
gf	-1239.39	kJ/mol	Joback Method
hf	-1562.94	kJ/mol	Joback Method
hfus	28.20	kJ/mol	Joback Method
hvap	51.63	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	4.927		Crippen Method
mcvol	202.420	ml/mol	McGowan Method
pc	1681.03	kPa	Joback Method
rinpol	1323.00		NIST Webbook
rinpol	1323.00		NIST Webbook
tb	621.37	K	Joback Method
tc	799.00	K	Joback Method
tf	364.54	K	Joback Method
vc	0.816	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	548.42	J/mol×K	621.37	Joback Method
cpg	562.04	J/mol×K	650.98	Joback Method
cpg	574.84	J/mol×K	680.58	Joback Method
cpg	586.84	J/mol×K	710.19	Joback Method
cpg	598.09	J/mol×K	739.79	Joback Method
cpg	608.63	J/mol×K	769.40	Joback Method
cpg	618.48	J/mol×K	799.00	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357363&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