2-Trifluoromethylbenzoic acid, 2-methylpentyl ester

Inchi: InChI=1S/C14H17F3O2/c1-3-6-10(2)9-19-13(18)11-7-4-5-8-12(11)14(15,16)17/h4-5,7-8,

InchiKey: DMMOPVJIZDICMU-UHFFFAOYSA-N

Formula: C14H17F3O2

SMILES: CCCC(C)COC(=O)c1ccccc1C(F)(F)F

Mol. weight [g/mol]: 274.28

Physical Properties

Property code	Value	Unit	Source
gf	-648.17	kJ/mol	Joback Method
hf	-954.39	kJ/mol	Joback Method
hfus	26.76	kJ/mol	Joback Method
hvap	54.72	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	4.298		Crippen Method
mcvol	197.110	ml/mol	McGowan Method
pc	1877.28	kPa	Joback Method
rinpol	1539.00		NIST Webbook
tb	621.81	K	Joback Method
tc	811.57	K	Joback Method
tf	347.83	K	Joback Method
vc	0.772	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.48	J/mol×K	621.81	Joback Method
cpg	536.52	J/mol×K	653.44	Joback Method
cpg	550.68	J/mol×K	685.06	Joback Method
cpg	563.99	J/mol×K	716.69	Joback Method
cpg	576.48	J/mol×K	748.32	Joback Method
cpg	588.18	J/mol×K	779.94	Joback Method
cpg	599.14	J/mol×K	811.57	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=U355154&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