2-Trifluoromethylbenzoic acid, 3-methylbutyl ester

Inchi: InChI=1S/C13H15F3O2/c1-9(2)7-8-18-12(17)10-5-3-4-6-11(10)13(14,15)16/h3-6,9H,7-8H

InchiKey: BQOOQUDGHPAWEX-UHFFFAOYSA-N

Formula: C13H15F3O2

SMILES: CC(C)CCOC(=O)c1ccccc1C(F)(F)F

Mol. weight [g/mol]: 260.25

Physical Properties

Property code	Value	Unit	Source
gf	-656.59	kJ/mol	Joback Method
hf	-933.75	kJ/mol	Joback Method
hfus	24.17	kJ/mol	Joback Method
hvap	52.49	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	3.908		Crippen Method
mcvol	183.020	ml/mol	McGowan Method
pc	2043.76	kPa	Joback Method
rinpol	1455.00		NIST Webbook
rinpol	1455.00		NIST Webbook
tb	598.93	K	Joback Method
tc	790.86	K	Joback Method
tf	336.56	K	Joback Method
vc	0.717	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	470.99	J/mol×K	598.93	Joback Method
cpg	485.54	J/mol×K	630.92	Joback Method
cpg	499.22	J/mol×K	662.91	Joback Method
cpg	512.08	J/mol×K	694.89	Joback Method
cpg	524.13	J/mol×K	726.88	Joback Method
cpg	535.41	J/mol×K	758.87	Joback Method
cpg	545.96	J/mol×K	790.86	Joback Method

Sources

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=U355152&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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