3-Trifluoromethylbenzoic acid, 3-methylbut-2-yl ester

Inchi: InChI=1S/C13H15F3O2/c1-8(2)9(3)18-12(17)10-5-4-6-11(7-10)13(14,15)16/h4-9H,1-3H3

InchiKey: FTQWVKYCCYWCIQ-UHFFFAOYSA-N

Formula: C13H15F3O2

SMILES: CC(C)C(C)OC(=O)c1cccc(C(F)(F)F)c1

Mol. weight [g/mol]: 260.25

Physical Properties

Property code	Value	Unit	Source
gf	-659.03	kJ/mol	Joback Method
hf	-939.03	kJ/mol	Joback Method
hfus	20.65	kJ/mol	Joback Method
hvap	52.10	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	3.907		Crippen Method
mcvol	183.020	ml/mol	McGowan Method
pc	2058.62	kPa	Joback Method
rinpol	1338.00		NIST Webbook
tb	598.49	K	Joback Method
tc	794.06	K	Joback Method
tf	321.56	K	Joback Method
vc	0.711	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	471.39	J/mol×K	598.49	Joback Method
cpg	486.27	J/mol×K	631.09	Joback Method
cpg	500.24	J/mol×K	663.68	Joback Method
cpg	513.33	J/mol×K	696.28	Joback Method
cpg	525.59	J/mol×K	728.87	Joback Method
cpg	537.05	J/mol×K	761.47	Joback Method
cpg	547.73	J/mol×K	794.06	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=U355137&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