3-Trifluoromethylbenzoic acid, 4-methoxy-2-methylbutyl ester

Inchi: InChI=1S/C14H17F3O3/c1-10(6-7-19-2)9-20-13(18)11-4-3-5-12(8-11)14(15,16)17/h3-5,8

InchiKey: OSKUTSBEHBXUIH-UHFFFAOYSA-N

Formula: C14H17F3O3

SMILES: COCCC(C)COC(=O)c1cccc(C(F)(F)F)c1

Mol. weight [g/mol]: 290.28

Physical Properties

Property code	Value	Unit	Source
gf	-753.17	kJ/mol	Joback Method
hf	-1086.61	kJ/mol	Joback Method
hfus	27.95	kJ/mol	Joback Method
hvap	57.13	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	3.535		Crippen Method
mcvol	202.980	ml/mol	McGowan Method
pc	1849.92	kPa	Joback Method
rinpol	1658.00		NIST Webbook
tb	644.23	K	Joback Method
tc	832.92	K	Joback Method
tf	370.06	K	Joback Method
vc	0.790	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	548.44	J/mol×K	644.23	Joback Method
cpg	563.14	J/mol×K	675.68	Joback Method
cpg	576.99	J/mol×K	707.13	Joback Method
cpg	590.01	J/mol×K	738.58	Joback Method
cpg	602.22	J/mol×K	770.02	Joback Method
cpg	613.66	J/mol×K	801.47	Joback Method
cpg	624.33	J/mol×K	832.92	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=U355142&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