2,3,4-Trifluorobenzoic acid, 3-methylbut-2-enyl ester

Inchi: InChI=1S/C12H11F3O2/c1-7(2)5-6-17-12(16)8-3-4-9(13)11(15)10(8)14/h3-5H,6H2,1-2H3

InchiKey: DIFDSKYIZZPOQX-UHFFFAOYSA-N

Formula: C12H11F3O2

SMILES: CC(C)=CCOC(=O)c1ccc(F)c(F)c1F

Mol. weight [g/mol]: 244.21

Physical Properties

Property code	Value	Unit	Source
gf	-613.00	kJ/mol	Joback Method
hf	-814.59	kJ/mol	Joback Method
hfus	30.63	kJ/mol	Joback Method
hvap	53.31	kJ/mol	Joback Method
log10ws	-4.24		Crippen Method
logp	3.227		Crippen Method
mcvol	164.630	ml/mol	McGowan Method
pc	2233.41	kPa	Joback Method
rinpol	1462.10		NIST Webbook
tb	593.72	K	Joback Method
tc	786.64	K	Joback Method
tf	343.87	K	Joback Method
vc	0.658	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	397.11	J/mol×K	593.72	Joback Method
cpg	409.27	J/mol×K	625.87	Joback Method
cpg	420.80	J/mol×K	658.03	Joback Method
cpg	431.71	J/mol×K	690.18	Joback Method
cpg	442.02	J/mol×K	722.33	Joback Method
cpg	451.75	J/mol×K	754.49	Joback Method
cpg	460.92	J/mol×K	786.64	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292552&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

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