Formic acid, (4-(trifluoromethoxy)phenyl)methyl ester

Inchi: InChI=1S/C9H7F3O3/c10-9(11,12)15-8-3-1-7(2-4-8)5-14-6-13/h1-4,6H,5H2
InchiKey: MVKBKJBJPHYVJC-UHFFFAOYSA-N
Formula: C9H7F3O3
SMILES: O=COCc1ccc(OC(F)(F)F)cc1
Mol. weight [g/mol]: 220.15

Physical Properties

Property code	Value	Unit	Source
gf	-763.43	kJ/mol	Joback Method
hf	-951.13	kJ/mol	Joback Method
hfus	19.21	kJ/mol	Joback Method
hvap	46.36	kJ/mol	Joback Method
log10ws	-2.91		Crippen Method
logp	2.258		Crippen Method
mcvol	132.530	ml/mol	McGowan Method
pc	2947.28	kPa	Joback Method
rinpol	1130.00		NIST Webbook
rinpol	1130.00		NIST Webbook
tb	525.06	K	Joback Method
tc	717.00	K	Joback Method
tf	320.78	K	Joback Method
vc	0.527	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	308.75	J/mol×K	525.06	Joback Method
cpg	319.55	J/mol×K	557.05	Joback Method
cpg	329.74	J/mol×K	589.04	Joback Method
cpg	339.33	J/mol×K	621.03	Joback Method
cpg	348.34	J/mol×K	653.02	Joback Method
cpg	356.78	J/mol×K	685.01	Joback Method
cpg	364.66	J/mol×K	717.00	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368954&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

Latest version available from:

https://www.chemeo.com/cid/24-604-4/Formic-acid-4-trifluoromethoxy-phenyl-methyl-ester.pdf

Generated by Cheméo on 2024-10-12 08:54:18.057581455 +0000 UTC m=+3304120.694550704.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.