Formic acid, (2-(trifluoromethyl)phenyl)methyl ester

Inchi: InChI=1S/C9H7F3O2/c10-9(11,12)8-4-2-1-3-7(8)5-14-6-13/h1-4,6H,5H2
InchiKey: KDIITQYLVWZKSH-UHFFFAOYSA-N
Formula: C9H7F3O2
SMILES: O=COCc1ccccc1C(F)(F)F
Mol. weight [g/mol]: 204.15

Physical Properties

Property code	Value	Unit	Source
gf	-658.43	kJ/mol	Joback Method
hf	-818.91	kJ/mol	Joback Method
hfus	18.02	kJ/mol	Joback Method
hvap	43.95	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	2.378		Crippen Method
mcvol	126.660	ml/mol	McGowan Method
pc	3002.44	kPa	Joback Method
rinpol	1114.00		NIST Webbook
tb	502.64	K	Joback Method
tc	695.94	K	Joback Method
tf	298.55	K	Joback Method
vc	0.509	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	285.99	J/mol×K	502.64	Joback Method
cpg	297.05	J/mol×K	534.86	Joback Method
cpg	307.44	J/mol×K	567.07	Joback Method
cpg	317.18	J/mol×K	599.29	Joback Method
cpg	326.29	J/mol×K	631.50	Joback Method
cpg	334.80	J/mol×K	663.72	Joback Method
cpg	342.73	J/mol×K	695.94	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=U368761&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