Acetic acid, 3,4,5-trifluorophenylmethyl ester

Inchi: InChI=1S/C9H7F3O2/c1-5(13)14-4-6-2-7(10)9(12)8(11)3-6/h2-3H,4H2,1H3
InchiKey: FYYUZOSXIUIKOX-UHFFFAOYSA-N
Formula: C9H7F3O2
SMILES: CC(=O)OCc1cc(F)c(F)c(F)c1
Mol. weight [g/mol]: 204.15

Physical Properties

Property code	Value	Unit	Source
gf	-709.93	kJ/mol	Joback Method
hf	-860.10	kJ/mol	Joback Method
hfus	23.97	kJ/mol	Joback Method
hvap	46.59	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	2.167		Crippen Method
mcvol	126.660	ml/mol	McGowan Method
pc	2814.34	kPa	Joback Method
rinpol	1169.00		NIST Webbook
rinpol	1169.00		NIST Webbook
tb	521.04	K	Joback Method
tc	709.89	K	Joback Method
tf	329.10	K	Joback Method
vc	0.509	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	280.60	J/mol×K	521.04	Joback Method
cpg	290.49	J/mol×K	552.51	Joback Method
cpg	299.95	J/mol×K	583.99	Joback Method
cpg	308.98	J/mol×K	615.46	Joback Method
cpg	317.58	J/mol×K	646.94	Joback Method
cpg	325.75	J/mol×K	678.41	Joback Method
cpg	333.50	J/mol×K	709.89	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=U367919&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

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