Acetic acid, trifluoro-, phenylmethyl ester

Other names:	Acetic acid, trifluoro-, benzyl ester
	Benzyl trifluoroacetate
	Trifluoroacetic acid, benzyl ester
	Benzenemethanol, trifluoroacetate
Inchi:	InChI=1S/C9H7F3O2/c10-9(11,12)8(13)14-6-7-4-2-1-3-5-7/h1-5H,6H2
InchiKey:	HDYQLGLEPPGPEV-UHFFFAOYSA-N
Formula:	C9H7F3O2
SMILES:	O=C(OCc1ccccc1)C(F)(F)F
Mol. weight [g/mol]:	204.15
CAS:	351-70-2

Physical Properties

Property code	Value	Unit	Source
gf	-678.20	kJ/mol	Joback Method
hf	-834.44	kJ/mol	Joback Method
hfus	17.72	kJ/mol	Joback Method
hvap	43.31	kJ/mol	Joback Method
log10ws	-2.71		Crippen Method
logp	2.292		Crippen Method
mcvol	126.660	ml/mol	McGowan Method
pc	3015.64	kPa	Joback Method
rinpol	988.00		NIST Webbook
rinpol	988.00		NIST Webbook
tb	502.87	K	Joback Method
tc	699.87	K	Joback Method
tf	293.96	K	Joback Method
vc	0.498	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	284.68	J/mol×K	502.87	Joback Method
cpg	296.41	J/mol×K	535.70	Joback Method
cpg	307.38	J/mol×K	568.54	Joback Method

cpg	317.62	J/mol×K	601.37	Joback Method
cpg	327.16	J/mol×K	634.20	Joback Method
cpg	336.03	J/mol×K	667.03	Joback Method
cpg	344.26	J/mol×K	699.87	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C351702&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