Acetic acid, trifluoro-, phenyl ester

Other names: Phenyl trifluoroacetate
Inchi: InChI=1S/C8H5F3O2/c9-8(10,11)7(12)13-6-4-2-1-3-5-6/h1-5H
InchiKey: DVCMYAIUSOSIQP-UHFFFAOYSA-N
Formula: C8H5F3O2
SMILES: O=C(Oc1ccccc1)C(F)(F)F
Mol. weight [g/mol]: 190.12
CAS: 500-73-2

Physical Properties

Property code	Value	Unit	Source
gf	-686.62	kJ/mol	Joback Method
hf	-813.80	kJ/mol	Joback Method
hfus	15.13	kJ/mol	Joback Method
hvap	41.09	kJ/mol	Joback Method
log10ws	-2.45		Crippen Method
logp	2.154		Crippen Method
mcvol	112.570	ml/mol	McGowan Method
pc	3360.64	kPa	Joback Method
rinpol	859.00		NIST Webbook
rinpol	859.00		NIST Webbook
tb	479.99	K	Joback Method
tc	679.57	K	Joback Method
tf	282.69	K	Joback Method
vc	0.443	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	242.57	J/mol×K	479.99	Joback Method
cpg	253.35	J/mol×K	513.25	Joback Method
cpg	263.40	J/mol×K	546.52	Joback Method
cpg	272.76	J/mol×K	579.78	Joback Method
cpg	281.46	J/mol×K	613.04	Joback Method
cpg	289.52	J/mol×K	646.30	Joback Method

cpg	296.98	J/mol×K	679.57	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=C500732&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