

Allyl trifluoroacetate

Other names:	Allyl trifluoroacetate Acetic acid, trifluoro-, 2-propenyl ester Acetic acid, trifluoro-, allyl ester Trifluoroacetic acid, 2-propenyl ester Allyl alcohol, trifluoroacetate
Inchi:	InChI=1S/C5H5F3O2/c1-2-3-10-4(9)5(6,7)8/h2H,1,3H2
InchiKey:	XIVPVSIDXBTZLM-UHFFFAOYSA-N
Formula:	C5H5F3O2
SMILES:	C=CCOC(=O)C(F)(F)F
Mol. weight [g/mol]:	154.09
CAS:	383-67-5

Physical Properties

Property code	Value	Unit	Source
gf	-736.45	kJ/mol	Joback Method
hf	-862.98	kJ/mol	Joback Method
hfus	12.04	kJ/mol	Joback Method
hvap	31.46	kJ/mol	Joback Method
log10ws	-1.29		Crippen Method
logp	1.278		Crippen Method
mcvol	89.760	ml/mol	McGowan Method
pc	3356.75	kPa	Joback Method
rinpol	708.30		NIST Webbook
rinpol	708.30		NIST Webbook
tb	381.35	K	Joback Method
tc	546.30	K	Joback Method
tf	220.70	K	Joback Method
vc	0.363	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	175.99	J/molxK	381.35	Joback Method
cpg	183.82	J/molxK	408.84	Joback Method

cpg	191.27	J/mol×K	436.33	Joback Method
cpg	198.35	J/mol×K	463.83	Joback Method
cpg	205.08	J/mol×K	491.32	Joback Method
cpg	211.46	J/mol×K	518.81	Joback Method
cpg	217.50	J/mol×K	546.30	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C383675&Units=SI

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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