Propargyl alcohol, trifluoroacetate

Inchi: InChI=1S/C5H3F3O2/c1-2-3-10-4(9)5(6,7)8/h1H,3H2
InchiKey: HJGKWNJPZJFBCJ-UHFFFAOYSA-N
Formula: C5H3F3O2
SMILES: C#CCOC(=O)C(F)(F)F
Mol. weight [g/mol]: 152.07

Physical Properties

Property code	Value	Unit	Source
gf	-601.22	kJ/mol	Joback Method
hf	-696.51	kJ/mol	Joback Method
hfus	16.29	kJ/mol	Joback Method
hvap	31.99	kJ/mol	Joback Method
log10ws	-1.24		Crippen Method
logp	0.725		Crippen Method
mcvol	85.460	ml/mol	McGowan Method
pc	3810.39	kPa	Joback Method
rinpol	711.00		NIST Webbook
rinpol	711.00		NIST Webbook
tb	374.79	K	Joback Method
tc	547.75	K	Joback Method
tf	269.43	K	Joback Method
vc	0.344	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	166.98	J/mol×K	374.79	Joback Method
cpg	173.76	J/mol×K	403.62	Joback Method
cpg	180.18	J/mol×K	432.44	Joback Method
cpg	186.23	J/mol×K	461.27	Joback Method
cpg	191.93	J/mol×K	490.10	Joback Method
cpg	197.31	J/mol×K	518.92	Joback Method
cpg	202.36	J/mol×K	547.75	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=U352283&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