Propargyl alcohol, pentafluoropropionate

Inchi: InChI=1S/C6H3F5O2/c1-2-3-13-4(12)5(7,8)6(9,10)11/h1H,3H2
InchiKey: XUOASYRZIYWGOG-UHFFFAOYSA-N
Formula: C6H3F5O2
SMILES: C#CCOC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 202.08

Physical Properties

Property code	Value	Unit	Source
gf	-979.58	kJ/mol	Joback Method
hf	-1118.12	kJ/mol	Joback Method
hfus	17.63	kJ/mol	Joback Method
hvap	31.29	kJ/mol	Joback Method
log10ws	-1.97		Crippen Method
logp	1.360		Crippen Method
mcvol	103.090	ml/mol	McGowan Method
pc	3131.49	kPa	Joback Method
rinpol	716.10		NIST Webbook
rinpol	716.10		NIST Webbook
tb	392.98	K	Joback Method
tc	557.86	K	Joback Method
tf	284.30	K	Joback Method
vc	0.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	219.91	J/mol×K	392.98	Joback Method
cpg	228.39	J/mol×K	420.46	Joback Method
cpg	236.32	J/mol×K	447.94	Joback Method
cpg	243.73	J/mol×K	475.42	Joback Method
cpg	250.65	J/mol×K	502.90	Joback Method
cpg	257.09	J/mol×K	530.38	Joback Method
cpg	263.09	J/mol×K	557.86	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352282&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

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