Propargyl alcohol, heptafluorobutyrate

Inchi: InChI=1S/C7H3F7O2/c1-2-3-16-4(15)5(8,9)6(10,11)7(12,13)14/h1H,3H2
InchiKey: SPKPBFWFVJVKJH-UHFFFAOYSA-N
Formula: C7H3F7O2
SMILES: C#CCOC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 252.09

Physical Properties

Property code	Value	Unit	Source
gf	-1357.94	kJ/mol	Joback Method
hf	-1539.73	kJ/mol	Joback Method
hfus	18.97	kJ/mol	Joback Method
hvap	30.58	kJ/mol	Joback Method
log10ws	-2.70		Crippen Method
logp	1.996		Crippen Method
mcvol	120.720	ml/mol	McGowan Method
pc	2619.09	kPa	Joback Method
rinpol	729.30		NIST Webbook
rinpol	729.30		NIST Webbook
tb	411.17	K	Joback Method
tc	568.71	K	Joback Method
tf	299.17	K	Joback Method
vc	0.506	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.69	J/mol×K	411.17	Joback Method
cpg	285.45	J/mol×K	437.43	Joback Method
cpg	294.54	J/mol×K	463.68	Joback Method
cpg	302.99	J/mol×K	489.94	Joback Method
cpg	310.84	J/mol×K	516.20	Joback Method
cpg	318.11	J/mol×K	542.45	Joback Method
cpg	324.83	J/mol×K	568.71	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352281&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume