Acetic acid, 2,2,3,4,4,4-hexafluorobutyl ester

Inchi: InChI=1S/C6H6F6O2/c1-3(13)14-2-5(8,9)4(7)6(10,11)12/h4H,2H2,1H3
InchiKey: HBRIAAIICOEFEL-UHFFFAOYSA-N
Formula: C6H6F6O2
SMILES: CC(=O)OCC(F)(F)C(F)C(F)(F)F
Mol. weight [g/mol]: 224.10

Physical Properties

Property code	Value	Unit	Source
gf	-1399.90	kJ/mol	Joback Method
hf	-1611.41	kJ/mol	Joback Method
hfus	14.21	kJ/mol	Joback Method
hvap	30.22	kJ/mol	Joback Method
log10ws	-2.14		Crippen Method
logp	2.085		Crippen Method
mcvol	113.460	ml/mol	McGowan Method
pc	2571.50	kPa	Joback Method
rinpol	721.00		NIST Webbook
rinpol	721.00		NIST Webbook
tb	401.69	K	Joback Method
tc	551.91	K	Joback Method
tf	222.92	K	Joback Method
vc	0.475	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	253.45	J/mol×K	401.69	Joback Method
cpg	263.16	J/mol×K	426.73	Joback Method
cpg	272.38	J/mol×K	451.76	Joback Method
cpg	281.12	J/mol×K	476.80	Joback Method
cpg	289.39	J/mol×K	501.83	Joback Method
cpg	297.22	J/mol×K	526.87	Joback Method
cpg	304.62	J/mol×K	551.91	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=U368914&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