Pentafluoropropionic acid, propyl ester

Other names: Propyl pentafluoropropanoate
Inchi: InChI=1S/C6H7F5O2/c1-2-3-13-4(12)5(7,8)6(9,10)11/h2-3H2,1H3
InchiKey: NZZLJQBPSUUZOQ-UHFFFAOYSA-N
Formula: C6H7F5O2
SMILES: CCCOC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 206.11

Physical Properties

Property code	Value	Unit	Source
gf	-1202.65	kJ/mol	Joback Method
hf	-1410.02	kJ/mol	Joback Method
hfus	14.65	kJ/mol	Joback Method
hvap	31.43	kJ/mol	Joback Method
log10ws	-2.17		Crippen Method
logp	2.137		Crippen Method
mcvol	111.690	ml/mol	McGowan Method
pc	2670.78	kPa	Joback Method
rinpol	592.00		NIST Webbook
rinpol	592.00		NIST Webbook
rinpol	592.00		NIST Webbook
tb	402.86	K	Joback Method
tc	557.50	K	Joback Method
tf	237.33	K	Joback Method
vc	0.464	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	245.22	J/mol×K	402.86	Joback Method
cpg	255.09	J/mol×K	428.63	Joback Method
cpg	264.44	J/mol×K	454.41	Joback Method
cpg	273.31	J/mol×K	480.18	Joback Method
cpg	281.70	J/mol×K	505.95	Joback Method
cpg	289.64	J/mol×K	531.73	Joback Method

cpg	297.14	J/mol×K	557.50	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=U355960&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