Heptafluorobutyric acid, propyl ester

Other names: Propyl heptafluorobutanoate
2,2,3,3,4,4,4-Heptafluoro-butyric acid propyl ester
Inchi: InChI=1S/C7H7F7O2/c1-2-3-16-4(15)5(8,9)6(10,11)7(12,13)14/h2-3H2,1H3
InchiKey: BBVCHFOOSHSLGN-UHFFFAOYSA-N
Formula: C7H7F7O2
SMILES: CCCOC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 256.12

Physical Properties

Property code	Value	Unit	Source
gf	-1581.01	kJ/mol	Joback Method
hf	-1831.63	kJ/mol	Joback Method
hfus	15.99	kJ/mol	Joback Method
hvap	30.73	kJ/mol	Joback Method
log10ws	-2.91		Crippen Method
logp	2.773		Crippen Method
mcvol	129.320	ml/mol	McGowan Method
pc	2263.26	kPa	Joback Method
rinpol	642.40		NIST Webbook
rinpol	671.00		NIST Webbook
rinpol	642.00		NIST Webbook
rinpol	642.00		NIST Webbook
tb	421.05	K	Joback Method
tc	569.35	K	Joback Method
tf	252.20	K	Joback Method
vc	0.544	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	303.12	J/mol×K	421.05	Joback Method
cpg	314.06	J/mol×K	445.77	Joback Method
cpg	324.38	J/mol×K	470.48	Joback Method
cpg	334.11	J/mol×K	495.20	Joback Method

cpg	343.27	J/mol×K	519.92	Joback Method
cpg	351.88	J/mol×K	544.64	Joback Method
cpg	359.97	J/mol×K	569.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355998&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