Pentafluoropropionic acid, butyl ester

Other names: Butyl pentafluoropropionate
Inchi: InChI=1S/C7H9F5O2/c1-2-3-4-14-5(13)6(8,9)7(10,11)12/h2-4H2,1H3
InchiKey: DUTTZBRMOIAYKM-UHFFFAOYSA-N
Formula: C7H9F5O2
SMILES: CCCCOC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 220.14
CAS: 680-28-4

Physical Properties

Property code	Value	Unit	Source
gf	-1194.23	kJ/mol	Joback Method
hf	-1430.66	kJ/mol	Joback Method
hfus	17.25	kJ/mol	Joback Method
hvap	33.66	kJ/mol	Joback Method
log10ws	-2.59		Crippen Method
logp	2.527		Crippen Method
mcvol	125.780	ml/mol	McGowan Method
pc	2424.27	kPa	Joback Method
rinpol	708.00		NIST Webbook
rinpol	685.00		NIST Webbook
rinpol	685.30		NIST Webbook
rinpol	685.00		NIST Webbook
rinpol	708.00		NIST Webbook
rinpol	687.00		NIST Webbook
ripol	760.00		NIST Webbook
ripol	760.00		NIST Webbook
tb	425.74	K	Joback Method
tc	580.14	K	Joback Method
tf	248.60	K	Joback Method
vc	0.519	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	284.60	J/mol×K	425.74	Joback Method
cpg	295.39	J/mol×K	451.47	Joback Method
cpg	305.64	J/mol×K	477.21	Joback Method
cpg	315.37	J/mol×K	502.94	Joback Method
cpg	324.59	J/mol×K	528.67	Joback Method
cpg	333.33	J/mol×K	554.40	Joback Method
cpg	341.60	J/mol×K	580.14	Joback Method
hvapt	38.60	kJ/mol	371.50	NIST Webbook

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=C680284&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
hvapt:	Enthalpy of vaporization at a given temperature
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume