4-Chlorobutyric acid, pentafluorophenyl ester

Inchi: InChI=1S/C10H6ClF5O2/c11-3-1-2-4(17)18-10-8(15)6(13)5(12)7(14)9(10)16/h1-3H2
InchiKey: OASWZKFZGUCTGJ-UHFFFAOYSA-N
Formula: C10H6ClF5O2
SMILES: O=C(CCCCl)Oc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 288.60

Physical Properties

Property code	Value	Unit	Source
gf	-1122.32	kJ/mol	Joback Method
hf	-1311.64	kJ/mol	Joback Method
hfus	36.14	kJ/mol	Joback Method
hvap	52.90	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	3.306		Crippen Method
mcvol	156.530	ml/mol	McGowan Method
pc	2187.68	kPa	Joback Method
rinpol	1366.00		NIST Webbook
rinpol	1369.00		NIST Webbook
rinpol	1366.00		NIST Webbook
tb	589.85	K	Joback Method
tc	767.28	K	Joback Method
tf	396.51	K	Joback Method
vc	0.650	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	363.77	J/mol×K	589.85	Joback Method
cpg	372.75	J/mol×K	619.42	Joback Method
cpg	381.34	J/mol×K	648.99	Joback Method
cpg	389.54	J/mol×K	678.56	Joback Method
cpg	397.35	J/mol×K	708.13	Joback Method
cpg	404.76	J/mol×K	737.71	Joback Method
cpg	411.77	J/mol×K	767.28	Joback Method

Sources

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=U360638&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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