4-Chlorobutyric acid, 2,2,3,3,4,4,5,5-octafluoropentyl ester

Inchi: InChI=1S/C9H9ClF8O2/c10-3-1-2-5(19)20-4-7(13,14)9(17,18)8(15,16)6(11)12/h6H,1-4H

InchiKey: NAZQCNNUKQMBEO-UHFFFAOYSA-N

Formula: C9H9ClF8O2

SMILES: O=C(CCCCl)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 336.61

Physical Properties

Property code	Value	Unit	Source
gf	-1773.35	kJ/mol	Joback Method
hf	-2090.04	kJ/mol	Joback Method
hfus	24.93	kJ/mol	Joback Method
hvap	38.36	kJ/mol	Joback Method
log10ws	-3.86		Crippen Method
logp	3.720		Crippen Method
mcvol	171.510	ml/mol	McGowan Method
pc	1783.35	kPa	Joback Method
rinpol	1213.00		NIST Webbook
rinpol	1193.00		NIST Webbook
tb	503.07	K	Joback Method
tc	653.32	K	Joback Method
tf	290.25	K	Joback Method
vc	0.718	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	427.63	J/mol×K	503.07	Joback Method
cpg	439.02	J/mol×K	528.11	Joback Method
cpg	449.74	J/mol×K	553.15	Joback Method
cpg	459.82	J/mol×K	578.20	Joback Method
cpg	469.30	J/mol×K	603.24	Joback Method
cpg	478.19	J/mol×K	628.28	Joback Method
cpg	486.54	J/mol×K	653.32	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=U360635&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