Butyl perfluorohexanoate

Other names: 2,2,3,3,4,4,5,5,6,6,6-Undecafluoro- hexanoic acid butyl ester
Inchi: InChI=1S/C10H9F11O2/c1-2-3-4-23-5(22)6(11,12)7(13,14)8(15,16)9(17,18)10(19,20)21/
InchiKey: LISFREFGRFFOEH-UHFFFAOYSA-N
Formula: C10H9F11O2
SMILES: CCCCOC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 370.16

Physical Properties

Property code	Value	Unit	Source
gf	-2329.31	kJ/mol	Joback Method
hf	-2695.49	kJ/mol	Joback Method
hfus	21.25	kJ/mol	Joback Method
hvap	31.54	kJ/mol	Joback Method
log10ws	-4.79		Crippen Method
logp	4.433		Crippen Method
mcvol	178.670	ml/mol	McGowan Method
pc	1559.81	kPa	Joback Method
rinpol	842.00		NIST Webbook
rinpol	842.20		NIST Webbook
tb	480.31	K	Joback Method
tc	618.73	K	Joback Method
tf	293.21	K	Joback Method
vc	0.762	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	471.73	J/mol×K	480.31	Joback Method
cpg	484.48	J/mol×K	503.38	Joback Method
cpg	496.45	J/mol×K	526.45	Joback Method
cpg	507.68	J/mol×K	549.52	Joback Method
cpg	518.20	J/mol×K	572.59	Joback Method
cpg	528.05	J/mol×K	595.66	Joback Method
cpg	537.27	J/mol×K	618.73	Joback Method

Sources

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=R70058&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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