Pentyl perfluorohexanoate

Other names: 2,2,3,3,4,4,5,5,6,6,6-Undecafluoro- hexanoic acid pentyl ester
Inchi: InChI=1S/C11H11F11O2/c1-2-3-4-5-24-6(23)7(12,13)8(14,15)9(16,17)10(18,19)11(20,21
InchiKey: HFOZGAUKNAKOOE-UHFFFAOYSA-N
Formula: C11H11F11O2
SMILES: CCCCCOC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 384.19

Physical Properties

Property code	Value	Unit	Source
gf	-2320.89	kJ/mol	Joback Method
hf	-2716.13	kJ/mol	Joback Method
hfus	23.84	kJ/mol	Joback Method
hvap	33.77	kJ/mol	Joback Method
log10ws	-5.21		Crippen Method
logp	4.823		Crippen Method
mcvol	192.760	ml/mol	McGowan Method
pc	1447.94	kPa	Joback Method
rinpol	935.60		NIST Webbook
rinpol	936.00		NIST Webbook
tb	503.19	K	Joback Method
tc	642.20	K	Joback Method
tf	304.48	K	Joback Method
vc	0.819	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	519.01	J/mol×K	503.19	Joback Method
cpg	532.16	J/mol×K	526.36	Joback Method
cpg	544.52	J/mol×K	549.53	Joback Method
cpg	556.14	J/mol×K	572.70	Joback Method
cpg	567.04	J/mol×K	595.87	Joback Method
cpg	577.26	J/mol×K	619.03	Joback Method
cpg	586.84	J/mol×K	642.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R70218&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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