Pentyl perfluoroheptanoate

Other names: 2,2,3,3,4,4,5,5,6,6,7,7,7-Tridecafluoro-heptanoic acid pentyl ester
Inchi: InChI=1S/C12H11F13O2/c1-2-3-4-5-27-6(26)7(13,14)8(15,16)9(17,18)10(19,20)11(21,22
InchiKey: QFCYZBVUAQZNQJ-UHFFFAOYSA-N
Formula: C12H11F13O2
SMILES: CCCCCOC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 434.19

Physical Properties

Property code	Value	Unit	Source
gf	-2699.25	kJ/mol	Joback Method
hf	-3137.74	kJ/mol	Joback Method
hfus	25.18	kJ/mol	Joback Method
hvap	33.06	kJ/mol	Joback Method
log10ws	-5.94		Crippen Method
logp	5.459		Crippen Method
mcvol	210.390	ml/mol	McGowan Method
pc	1280.08	kPa	Joback Method
rinpol	991.00		NIST Webbook
rinpol	991.40		NIST Webbook
rinpol	991.00		NIST Webbook
tb	521.38	K	Joback Method
tc	657.28	K	Joback Method
tf	319.35	K	Joback Method
vc	0.899	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	586.69	J/mol×K	521.38	Joback Method
cpg	600.06	J/mol×K	544.03	Joback Method
cpg	612.60	J/mol×K	566.68	Joback Method
cpg	624.36	J/mol×K	589.33	Joback Method
cpg	635.36	J/mol×K	611.98	Joback Method
cpg	645.65	J/mol×K	634.63	Joback Method

cpg	655.27	J/mol×K	657.28	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R70204&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

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