Pentadecafluorooctanoic acid, 4-chlorophenyl ester

Inchi: InChI=1S/C14H4ClF15O2/c15-5-1-3-6(4-2-5)32-7(31)8(16,17)9(18,19)10(20,21)11(22,23

InchiKey: PXASKELRUZCUSF-UHFFFAOYSA-N

Formula: C14H4ClF15O2

SMILES: O=C(Oc1ccc(Cl)cc1)C(F)(F)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]: 524.61

Physical Properties

Property code	Value	Unit	Source
gf	-2978.34	kJ/mol	Joback Method
hf	-3370.67	kJ/mol	Joback Method
hfus	26.95	kJ/mol	Joback Method
hvap	41.91	kJ/mol	Joback Method
log10ws	-7.53		Crippen Method
logp	6.619		Crippen Method
mcvol	230.590	ml/mol	McGowan Method
pc	1294.86	kPa	Joback Method
rinpol	1274.00		NIST Webbook
rinpol	1274.00		NIST Webbook
tb	631.54	K	Joback Method
tc	792.87	K	Joback Method
tf	414.35	K	Joback Method
vc	0.978	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	665.19	J/mol×K	631.54	Joback Method
cpg	675.80	J/mol×K	658.43	Joback Method
cpg	685.43	J/mol×K	685.32	Joback Method
cpg	694.16	J/mol×K	712.20	Joback Method
cpg	702.06	J/mol×K	739.09	Joback Method
cpg	709.21	J/mol×K	765.98	Joback Method
cpg	715.70	J/mol×K	792.87	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406892&Units=SI

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

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