Pentadecafluorooctanoic acid, 8-chlorooctyl ester

Inchi: InChI=1S/C16H16ClF15O2/c17-7-5-3-1-2-4-6-8-34-9(33)10(18,19)11(20,21)12(22,23)13

InchiKey: SJEQZDCUDPWWAO-UHFFFAOYSA-N

Formula: C16H16ClF15O2

SMILES: O=C(OCCCCCCCCCl)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]: 560.73

Physical Properties

Property code	Value	Unit	Source
gf	-3064.28	kJ/mol	Joback Method
hf	-3637.01	kJ/mol	Joback Method
hfus	38.48	kJ/mol	Joback Method
hvap	43.42	kJ/mol	Joback Method
log10ws	-8.08		Crippen Method
logp	7.483		Crippen Method
mcvol	282.530	ml/mol	McGowan Method
pc	925.55	kPa	Joback Method
rinpol	1551.00		NIST Webbook
rinpol	1551.00		NIST Webbook
tb	645.64	K	Joback Method
tc	793.13	K	Joback Method
tf	397.95	K	Joback Method
vc	1.198	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	846.65	J/mol×K	645.64	Joback Method
cpg	860.05	J/mol×K	670.22	Joback Method
cpg	872.53	J/mol×K	694.80	Joback Method
cpg	884.16	J/mol×K	719.39	Joback Method
cpg	895.01	J/mol×K	743.97	Joback Method
cpg	905.14	J/mol×K	768.55	Joback Method
cpg	914.61	J/mol×K	793.13	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=U406812&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