Pentadecafluorooctanoic acid, cyclohexylmethyl ester

Inchi: InChI=1S/C15H13F15O2/c16-9(17,8(31)32-6-7-4-2-1-3-5-7)10(18,19)11(20,21)12(22,23)
InchiKey: QOGLORBQBFFERD-UHFFFAOYSA-N
Formula: C15H13F15O2
SMILES: O=C(OCC1CCCCC1)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]: 510.24

Physical Properties

Property code	Value	Unit	Source
gf	-3036.32	kJ/mol	Joback Method
hf	-3546.31	kJ/mol	Joback Method
hfus	23.53	kJ/mol	Joback Method
hvap	37.24	kJ/mol	Joback Method
log10ws	-7.16		Crippen Method
logp	6.484		Crippen Method
mcvol	245.340	ml/mol	McGowan Method
pc	1149.87	kPa	Joback Method
rinpol	1243.00		NIST Webbook
tb	604.88	K	Joback Method
tc	756.99	K	Joback Method
tf	364.14	K	Joback Method
vc	1.026	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	752.18	J/mol×K	604.88	Joback Method
cpg	767.67	J/mol×K	630.23	Joback Method
cpg	782.05	J/mol×K	655.58	Joback Method
cpg	795.39	J/mol×K	680.93	Joback Method
cpg	807.74	J/mol×K	706.28	Joback Method
cpg	819.18	J/mol×K	731.63	Joback Method
cpg	829.79	J/mol×K	756.99	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406810&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