Pentadecafluorooctanoic acid, oct-3-en-2-yl ester

Inchi: InChI=1S/C16H15F15O2/c1-3-4-5-6-7-8(2)33-9(32)10(17,18)11(19,20)12(21,22)13(23,24

InchiKey: YTNCTWJYJGADOP-VOTSOKGWSA-N

Formula: C16H15F15O2

SMILES: CCCCC=CC(C)OC(=O)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]: 524.27

Physical Properties

Property code	Value	Unit	Source
gf	-2974.57	kJ/mol	Joback Method
hf	-3509.33	kJ/mol	Joback Method
hfus	30.96	kJ/mol	Joback Method
hvap	38.61	kJ/mol	Joback Method
log10ws	-7.89		Crippen Method
logp	7.039		Crippen Method
mcvol	265.990	ml/mol	McGowan Method
pc	982.69	kPa	Joback Method
rinpol	1215.00		NIST Webbook
rinpol	1215.00		NIST Webbook
tb	611.93	K	Joback Method
tc	756.21	K	Joback Method
tf	347.95	K	Joback Method
vc	1.123	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	793.38	J/mol×K	611.93	Joback Method
cpg	807.35	J/mol×K	635.98	Joback Method
cpg	820.36	J/mol×K	660.02	Joback Method
cpg	832.49	J/mol×K	684.07	Joback Method
cpg	843.79	J/mol×K	708.12	Joback Method
cpg	854.33	J/mol×K	732.17	Joback Method
cpg	864.17	J/mol×K	756.21	Joback Method

Sources

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=U406923&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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