Pentadecafluorooctanoic acid, undec-2-en-1-yl ester

Inchi: InChI=1S/C19H21F15O2/c1-2-3-4-5-6-7-8-9-10-11-36-12(35)13(20,21)14(22,23)15(24,25

InchiKey: KWQWVJBGFXFMEX-MDZDMXLPSA-N

Formula: C19H21F15O2

SMILES: CCCCCCCCC=CCOC(=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]: 566.34

Physical Properties

Property code	Value	Unit	Source
gf	-2946.87	kJ/mol	Joback Method
hf	-3565.97	kJ/mol	Joback Method
hfus	42.26	kJ/mol	Joback Method
hvap	45.67	kJ/mol	Joback Method
log10ws	-9.04		Crippen Method
logp	8.211		Crippen Method
mcvol	308.260	ml/mol	McGowan Method
pc	822.90	kPa	Joback Method
rinpol	1543.00		NIST Webbook
tb	681.01	K	Joback Method
tc	834.30	K	Joback Method
tf	396.76	K	Joback Method
vc	1.296	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	957.24	J/mol×K	681.01	Joback Method
cpg	972.12	J/mol×K	706.56	Joback Method
cpg	986.02	J/mol×K	732.11	Joback Method
cpg	999.03	J/mol×K	757.65	Joback Method
cpg	1011.22	J/mol×K	783.20	Joback Method
cpg	1022.68	J/mol×K	808.75	Joback Method
cpg	1033.47	J/mol×K	834.30	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=U406926&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