Pentadecafluorooctanoic acid, 2,7-dimethyloct-1-en-3-yn-5-yl ester

Inchi: InChI=1S/C18H15F15O2/c1-8(2)5-6-10(7-9(3)4)35-11(34)12(19,20)13(21,22)14(23,24)15

InchiKey: NFZUCRFRZSIQAT-UHFFFAOYSA-N

Formula: C18H15F15O2

SMILES: C=C(C)C#CC(CC(C)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]: 548.29

Physical Properties

Property code	Value	Unit	Source
gf	-2758.30	kJ/mol	Joback Method
hf	-3285.17	kJ/mol	Joback Method
hfus	32.95	kJ/mol	Joback Method
hvap	44.28	kJ/mol	Joback Method
log10ws	-8.28		Crippen Method
logp	6.898		Crippen Method
mcvol	285.570	ml/mol	McGowan Method
pc	965.07	kPa	Joback Method
rinpol	1277.00		NIST Webbook
tb	658.65	K	Joback Method
tc	815.06	K	Joback Method
tf	450.95	K	Joback Method
vc	1.192	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	858.57	J/mol×K	658.65	Joback Method
cpg	872.33	J/mol×K	684.72	Joback Method
cpg	885.10	J/mol×K	710.79	Joback Method
cpg	896.96	J/mol×K	736.85	Joback Method
cpg	907.98	J/mol×K	762.92	Joback Method
cpg	918.25	J/mol×K	788.99	Joback Method
cpg	927.84	J/mol×K	815.06	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406925&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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