Pentadecafluorooctanoic acid, 2-methyloct-5-en-4-yl ester

Inchi: InChI=1S/C17H15F15O2/c1-4-5-6-9(7-8(2)3)34-10(33)11(18,19)12(20,21)13(22,23)14(24

InchiKey: RUTBYSRAPVHJGT-UHFFFAOYSA-N

Formula: C17H15F15O2

SMILES: CCC#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]: 536.28

Physical Properties

Property code	Value	Unit	Source
gf	-2846.01	kJ/mol	Joback Method
hf	-3380.17	kJ/mol	Joback Method
hfus	32.95	kJ/mol	Joback Method
hvap	42.64	kJ/mol	Joback Method
log10ws	-8.01		Crippen Method
logp	6.732		Crippen Method
mcvol	275.780	ml/mol	McGowan Method
pc	995.13	kPa	Joback Method
rinpol	1244.00		NIST Webbook
rinpol	1244.00		NIST Webbook
tb	639.21	K	Joback Method
tc	791.77	K	Joback Method
tf	455.40	K	Joback Method
vc	1.155	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	827.73	J/mol×K	639.21	Joback Method
cpg	841.66	J/mol×K	664.64	Joback Method
cpg	854.61	J/mol×K	690.06	Joback Method
cpg	866.66	J/mol×K	715.49	Joback Method
cpg	877.87	J/mol×K	740.92	Joback Method
cpg	888.31	J/mol×K	766.34	Joback Method
cpg	898.05	J/mol×K	791.77	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=U406924&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

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