Pentadecafluorooctanoic acid, hex-4-yn-3-yl ester

Inchi: InChI=1S/C14H9F15O2/c1-3-5-6(4-2)31-7(30)8(15,16)9(17,18)10(19,20)11(21,22)12(23,

InchiKey: WIUXGCBDNKBVII-UHFFFAOYSA-N

Formula: C14H9F15O2

SMILES: CC#CC(CC)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]: 494.20

Physical Properties

Property code	Value	Unit	Source
gf	-2868.83	kJ/mol	Joback Method
hf	-3312.97	kJ/mol	Joback Method
hfus	28.70	kJ/mol	Joback Method
hvap	36.35	kJ/mol	Joback Method
log10ws	-7.00		Crippen Method
logp	5.706		Crippen Method
mcvol	233.510	ml/mol	McGowan Method
pc	1197.30	kPa	Joback Method
rinpol	1079.00		NIST Webbook
rinpol	1079.00		NIST Webbook
tb	571.01	K	Joback Method
tc	718.02	K	Joback Method
tf	436.59	K	Joback Method
vc	0.993	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	671.03	J/mol×K	571.01	Joback Method
cpg	684.06	J/mol×K	595.51	Joback Method
cpg	696.14	J/mol×K	620.01	Joback Method
cpg	707.33	J/mol×K	644.52	Joback Method
cpg	717.68	J/mol×K	669.02	Joback Method
cpg	727.25	J/mol×K	693.52	Joback Method
cpg	736.09	J/mol×K	718.02	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406808&Units=SI

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