Pentadecafluorooctanoic acid, 2-methylpent-3-yl ester

Inchi: InChI=1S/C14H13F15O2/c1-4-6(5(2)3)31-7(30)8(15,16)9(17,18)10(19,20)11(21,22)12(23

InchiKey: LZAPIGSUVTWSOH-UHFFFAOYSA-N

Formula: C14H13F15O2

SMILES: CCC(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)C(C)C

Mol. weight [g/mol]: 498.23

Physical Properties

Property code	Value	Unit	Source
gf	-3074.07	kJ/mol	Joback Method
hf	-3590.55	kJ/mol	Joback Method
hfus	22.06	kJ/mol	Joback Method
hvap	33.81	kJ/mol	Joback Method
log10ws	-6.96		Crippen Method
logp	6.338		Crippen Method
mcvol	242.110	ml/mol	McGowan Method
pc	1080.64	kPa	Joback Method
rinpol	1038.00		NIST Webbook
rinpol	1038.00		NIST Webbook
tb	561.57	K	Joback Method
tc	699.92	K	Joback Method
tf	315.49	K	Joback Method
vc	1.024	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	707.52	J/mol×K	561.57	Joback Method
cpg	721.71	J/mol×K	584.63	Joback Method
cpg	734.97	J/mol×K	607.69	Joback Method
cpg	747.35	J/mol×K	630.75	Joback Method
cpg	758.90	J/mol×K	653.80	Joback Method
cpg	769.67	J/mol×K	676.86	Joback Method
cpg	779.71	J/mol×K	699.92	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=U406805&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