Pentadecafluorooctanoic acid, 3-methylbut-2-en-1-yl ester

Inchi: InChI=1S/C13H9F15O2/c1-5(2)3-4-30-6(29)7(14,15)8(16,17)9(18,19)10(20,21)11(22,23)

InchiKey: BXNSQBSBFPIMEZ-UHFFFAOYSA-N

Formula: C13H9F15O2

SMILES: CC(C)=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]: 482.19

Physical Properties

Property code	Value	Unit	Source
gf	-3005.94	kJ/mol	Joback Method
hf	-3451.92	kJ/mol	Joback Method
hfus	25.41	kJ/mol	Joback Method
hvap	32.40	kJ/mol	Joback Method
log10ws	-6.53		Crippen Method
logp	5.870		Crippen Method
mcvol	223.720	ml/mol	McGowan Method
pc	1184.97	kPa	Joback Method
rinpol	1131.00		NIST Webbook
rinpol	1131.00		NIST Webbook
tb	543.61	K	Joback Method
tc	682.52	K	Joback Method
tf	315.18	K	Joback Method
vc	0.962	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	637.62	J/mol×K	543.61	Joback Method
cpg	650.78	J/mol×K	566.76	Joback Method
cpg	663.01	J/mol×K	589.91	Joback Method
cpg	674.36	J/mol×K	613.07	Joback Method
cpg	684.89	J/mol×K	636.22	Joback Method
cpg	694.63	J/mol×K	659.37	Joback Method
cpg	703.66	J/mol×K	682.52	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406806&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

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