Pentadecafluorooctanoic acid, 3-methylbut-2-yl ester

Inchi: InChI=1S/C13H11F15O2/c1-4(2)5(3)30-6(29)7(14,15)8(16,17)9(18,19)10(20,21)11(22,23

InchiKey: IHUFQUGUZNPEEO-UHFFFAOYSA-N

Formula: C13H11F15O2

SMILES: CC(C)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]: 484.20

Physical Properties

Property code	Value	Unit	Source
gf	-3082.49	kJ/mol	Joback Method
hf	-3569.91	kJ/mol	Joback Method
hfus	19.47	kJ/mol	Joback Method
hvap	31.58	kJ/mol	Joback Method
log10ws	-6.54		Crippen Method
logp	5.948		Crippen Method
mcvol	228.020	ml/mol	McGowan Method
pc	1152.22	kPa	Joback Method
rinpol	972.00		NIST Webbook
rinpol	972.00		NIST Webbook
tb	538.69	K	Joback Method
tc	675.53	K	Joback Method
tf	304.22	K	Joback Method
vc	0.969	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	656.13	J/mol×K	538.69	Joback Method
cpg	670.09	J/mol×K	561.50	Joback Method
cpg	683.12	J/mol×K	584.30	Joback Method
cpg	695.27	J/mol×K	607.11	Joback Method
cpg	706.60	J/mol×K	629.92	Joback Method
cpg	717.14	J/mol×K	652.73	Joback Method
cpg	726.96	J/mol×K	675.53	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=U406804&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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