Pentadecafluorooctanoic acid, isobutyl ester

Inchi: InChI=1S/C12H9F15O2/c1-4(2)3-29-5(28)6(13,14)7(15,16)8(17,18)9(19,20)10(21,22)11(
InchiKey: WRMQEARPYRLONJ-UHFFFAOYSA-N
Formula: C12H9F15O2
SMILES: CC(C)COC(=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]: 470.17

Physical Properties

Property code	Value	Unit	Source
gf	-3088.47	kJ/mol	Joback Method
hf	-3543.99	kJ/mol	Joback Method
hfus	20.40	kJ/mol	Joback Method
hvap	29.75	kJ/mol	Joback Method
log10ws	-6.01		Crippen Method
logp	5.560		Crippen Method
mcvol	213.930	ml/mol	McGowan Method
pc	1224.27	kPa	Joback Method
rinpol	934.00		NIST Webbook
rinpol	934.00		NIST Webbook
tb	516.25	K	Joback Method
tc	650.14	K	Joback Method
tf	307.95	K	Joback Method
vc	0.918	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	605.73	J/mol×K	516.25	Joback Method
cpg	619.22	J/mol×K	538.56	Joback Method
cpg	631.82	J/mol×K	560.88	Joback Method
cpg	643.57	J/mol×K	583.19	Joback Method
cpg	654.51	J/mol×K	605.51	Joback Method
cpg	664.70	J/mol×K	627.82	Joback Method
cpg	674.18	J/mol×K	650.14	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406032&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