Heptadecafluorononanoic acid, butyl ester

Inchi: InChI=1S/C13H9F17O2/c1-2-3-4-32-5(31)6(14,15)7(16,17)8(18,19)9(20,21)10(22,23)11(
InchiKey: FDPTXAYZTQYILM-UHFFFAOYSA-N
Formula: C13H9F17O2
SMILES: CCCCOC(=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)C(F)(F)F
Mol. weight [g/mol]: 520.18

Physical Properties

Property code	Value	Unit	Source
gf	-3464.39	kJ/mol	Joback Method
hf	-3960.32	kJ/mol	Joback Method
hfus	25.26	kJ/mol	Joback Method
hvap	29.43	kJ/mol	Joback Method
log10ws	-6.99		Crippen Method
logp	6.339		Crippen Method
mcvol	231.560	ml/mol	McGowan Method
pc	1087.06	kPa	Joback Method
rinpol	1001.00		NIST Webbook
rinpol	1001.00		NIST Webbook
tb	534.88	K	Joback Method
tc	665.54	K	Joback Method
tf	337.82	K	Joback Method
vc	1.006	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	674.53	J/mol×K	534.88	Joback Method
cpg	687.94	J/mol×K	556.66	Joback Method
cpg	700.45	J/mol×K	578.43	Joback Method
cpg	712.10	J/mol×K	600.21	Joback Method
cpg	722.94	J/mol×K	621.99	Joback Method
cpg	733.02	J/mol×K	643.77	Joback Method
cpg	742.37	J/mol×K	665.54	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356019&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

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