Heptadecafluorononanoic acid, methyl ester

Inchi: InChI=1S/C10H3F17O2/c1-29-2(28)3(11,12)4(13,14)5(15,16)6(17,18)7(19,20)8(21,22)9(
InchiKey: CFNCFMKWDPDIPT-UHFFFAOYSA-N
Formula: C10H3F17O2
SMILES: 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)C(F)(F)F
Mol. weight [g/mol]: 478.10

Physical Properties

Property code	Value	Unit	Source
gf	-3489.65	kJ/mol	Joback Method
hf	-3898.40	kJ/mol	Joback Method
hfus	17.49	kJ/mol	Joback Method
hvap	22.75	kJ/mol	Joback Method
log10ws	-5.73		Crippen Method
logp	5.169		Crippen Method
mcvol	189.290	ml/mol	McGowan Method
pc	1327.14	kPa	Joback Method
rinpol	760.50		NIST Webbook
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tb	466.24	K	Joback Method
tc	592.08	K	Joback Method
tf	304.01	K	Joback Method
vc	0.838	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	527.50	J/mol×K	466.24	Joback Method
cpg	540.26	J/mol×K	487.21	Joback Method
cpg	552.13	J/mol×K	508.19	Joback Method
cpg	563.17	J/mol×K	529.16	Joback Method
cpg	573.41	J/mol×K	550.13	Joback Method
cpg	582.88	J/mol×K	571.11	Joback Method
cpg	591.64	J/mol×K	592.08	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352528&Units=SI

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