Octanoic acid, pentadecafluoro-, methyl ester

Other names:	Methyl perfluorooctanoate
	Pentadecafluorooctanoic acid, methyl ester
	Methylpentadecafluorooctanoate
	Octanoic acid, perfluoro-, methyl ester
Inchi:	InChI=1S/C9H3F15O2/c1-26-2(25)3(10,11)4(12,13)5(14,15)6(16,17)7(18,19)8(20,21)9(2
InchiKey:	XOCNYZFAMHDXJK-UHFFFAOYSA-N
Formula:	C9H3F15O2
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)F
Mol. weight [g/mol]:	428.10
CAS:	376-27-2

Physical Properties

Property code	Value	Unit	Source
gf	-3111.29	kJ/mol	Joback Method
hf	-3476.79	kJ/mol	Joback Method
hfus	16.16	kJ/mol	Joback Method
hvap	23.46	kJ/mol	Joback Method
log10ws	-5.00		Crippen Method
logp	4.534		Crippen Method
mcvol	171.660	ml/mol	McGowan Method
pc	1504.65	kPa	Joback Method
rinpol	549.00		NIST Webbook
tb	431.50 ± 0.50	K	NIST Webbook
tc	576.84	K	Joback Method
tf	289.14	K	Joback Method
vc	0.756	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	462.84	J/mol×K	448.05	Joback Method
cpg	475.27	J/mol×K	469.52	Joback Method
cpg	486.85	J/mol×K	490.98	Joback Method
cpg	497.63	J/mol×K	512.45	Joback Method

cpg	507.64	J/mol×K	533.91	Joback Method
cpg	516.92	J/mol×K	555.38	Joback Method
cpg	525.51	J/mol×K	576.84	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=C376272&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