Methyl 9H-perfluorononanoate

Inchi: InChI=1S/C10H4F16O2/c1-28-3(27)5(15,16)7(19,20)9(23,24)10(25,26)8(21,22)6(17,18)4
InchiKey: DAAHZPCZVKQFFH-UHFFFAOYSA-N
Formula: C10H4F16O2
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
Mol. weight [g/mol]: 460.11

Physical Properties

Property code	Value	Unit	Source
gf	-3300.12	kJ/mol	Joback Method
hf	-3698.82	kJ/mol	Joback Method
hfus	18.30	kJ/mol	Joback Method
hvap	24.48	kJ/mol	Joback Method
log10ws	-5.38		Crippen Method
logp	4.872		Crippen Method
mcvol	187.520	ml/mol	McGowan Method
pc	1360.63	kPa	Joback Method
rinpol	708.00		NIST Webbook
tb	469.76	K	Joback Method
tc	596.91	K	Joback Method
tf	286.00	K	Joback Method
vc	0.825	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	517.28	J/mol×K	469.76	Joback Method
cpg	529.84	J/mol×K	490.95	Joback Method
cpg	541.58	J/mol×K	512.14	Joback Method
cpg	552.52	J/mol×K	533.34	Joback Method
cpg	562.71	J/mol×K	554.53	Joback Method
cpg	572.18	J/mol×K	575.72	Joback Method
cpg	580.97	J/mol×K	596.91	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R385941&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