Methyl 7H-perfluoroheptanoate

Inchi: InChI=1S/C8H4F12O2/c1-22-3(21)5(13,14)7(17,18)8(19,20)6(15,16)4(11,12)2(9)10/h2H,
InchiKey: OJPGHRSOBKDLSK-UHFFFAOYSA-N
Formula: C8H4F12O2
SMILES: COC(=O)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]: 360.10

Physical Properties

Property code	Value	Unit	Source
gf	-2543.40	kJ/mol	Joback Method
hf	-2855.60	kJ/mol	Joback Method
hfus	15.63	kJ/mol	Joback Method
hvap	25.89	kJ/mol	Joback Method
log10ws	-3.92		Crippen Method
logp	3.601		Crippen Method
mcvol	152.260	ml/mol	McGowan Method
pc	1769.87	kPa	Joback Method
rinpol	614.00		NIST Webbook
tb	433.38	K	Joback Method
tc	567.49	K	Joback Method
tf	256.26	K	Joback Method
vc	0.662	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	390.06	J/mol×K	433.38	Joback Method
cpg	401.73	J/mol×K	455.73	Joback Method
cpg	412.66	J/mol×K	478.08	Joback Method
cpg	422.89	J/mol×K	500.44	Joback Method
cpg	432.46	J/mol×K	522.79	Joback Method
cpg	441.38	J/mol×K	545.14	Joback Method
cpg	449.69	J/mol×K	567.49	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R385936&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