Methyl perfluoroheptanoate

Other names: 2,2,3,3,4,4,5,5,6,6,7,7,7-Tridecafluoro-heptanoic acid methyl ester
Inchi: InChI=1S/C8H3F13O2/c1-23-2(22)3(9,10)4(11,12)5(13,14)6(15,16)7(17,18)8(19,20)21/h
InchiKey: JHROQORAJUWVCD-UHFFFAOYSA-N
Formula: C8H3F13O2
SMILES: COC(=O)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]: 378.09

Physical Properties

Property code	Value	Unit	Source
gf	-2732.93	kJ/mol	Joback Method
hf	-3055.18	kJ/mol	Joback Method
hfus	14.82	kJ/mol	Joback Method
hvap	24.16	kJ/mol	Joback Method
log10ws	-4.27		Crippen Method
logp	3.898		Crippen Method
mcvol	154.030	ml/mol	McGowan Method
pc	1720.31	kPa	Joback Method
rinpol	653.20		NIST Webbook
rinpol	653.00		NIST Webbook
tb	429.86	K	Joback Method
tc	562.41	K	Joback Method
tf	274.27	K	Joback Method
vc	0.675	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	400.08	J/mol×K	429.86	Joback Method
cpg	412.04	J/mol×K	451.95	Joback Method
cpg	423.20	J/mol×K	474.04	Joback Method
cpg	433.61	J/mol×K	496.13	Joback Method
cpg	443.28	J/mol×K	518.23	Joback Method
cpg	452.26	J/mol×K	540.32	Joback Method
cpg	460.58	J/mol×K	562.41	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=R70165&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