Methyl perfluorodecanoate

Inchi: InChI=1S/C11H3F19O2/c1-32-2(31)3(12,13)4(14,15)5(16,17)6(18,19)7(20,21)8(22,23)9(
InchiKey: QJFHNYDPNSFJMR-UHFFFAOYSA-N
Formula: C11H3F19O2
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)C(F)(F)F
Mol. weight [g/mol]: 528.11

Physical Properties

Property code	Value	Unit	Source
gf	-3868.01	kJ/mol	Joback Method
hf	-4320.01	kJ/mol	Joback Method
hfus	18.83	kJ/mol	Joback Method
hvap	22.05	kJ/mol	Joback Method
log10ws	-6.46		Crippen Method
logp	5.804		Crippen Method
mcvol	206.920	ml/mol	McGowan Method
pc	1179.28	kPa	Joback Method
rinpol	638.00		NIST Webbook
tb	484.43	K	Joback Method
tc	608.18	K	Joback Method
tf	318.88	K	Joback Method
vc	0.918	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	593.83	J/mol×K	484.43	Joback Method
cpg	606.82	J/mol×K	505.05	Joback Method
cpg	618.90	J/mol×K	525.68	Joback Method
cpg	630.10	J/mol×K	546.30	Joback Method
cpg	640.48	J/mol×K	566.93	Joback Method
cpg	650.06	J/mol×K	587.55	Joback Method
cpg	658.90	J/mol×K	608.18	Joback Method

Sources

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=R385956&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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