Ethyl perfluoroheptanoate

Other names: 2,2,3,3,4,4,5,5,6,6,7,7,7-Tridecafluoro-heptanoic acid ethyl ester
Inchi: InChI=1S/C9H5F13O2/c1-2-24-3(23)4(10,11)5(12,13)6(14,15)7(16,17)8(18,19)9(20,21)2
InchiKey: ZESCSNXJAROIJS-UHFFFAOYSA-N
Formula: C9H5F13O2
SMILES: CCOC(=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]: 392.11
CAS: 41430-70-0

Physical Properties

Property code	Value	Unit	Source
gf	-2724.51	kJ/mol	Joback Method
hf	-3075.82	kJ/mol	Joback Method
hfus	17.41	kJ/mol	Joback Method
hvap	26.39	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	4.288		Crippen Method
mcvol	168.120	ml/mol	McGowan Method
pc	1591.08	kPa	Joback Method
rinpol	724.00		NIST Webbook
rinpol	723.80		NIST Webbook
tb	452.74	K	Joback Method
tc	585.98	K	Joback Method
tf	285.54	K	Joback Method
vc	0.732	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	444.51	J/mol×K	452.74	Joback Method
cpg	456.86	J/mol×K	474.95	Joback Method
cpg	468.40	J/mol×K	497.15	Joback Method
cpg	479.18	J/mol×K	519.36	Joback Method
cpg	489.22	J/mol×K	541.57	Joback Method
cpg	498.57	J/mol×K	563.77	Joback Method

cpg	507.25	J/mol×K	585.98	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=C41430700&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