1H-Perfluoroheptane

Inchi: InChI=1S/C7HF15/c8-1(9)2(10,11)3(12,13)4(14,15)5(16,17)6(18,19)7(20,21)22/h1H
InchiKey: HBZVXKDQRIQMCW-UHFFFAOYSA-N
Formula: C7HF15
SMILES: FC(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 370.06
CAS: 27213-61-2

Physical Properties

Property code	Value	Unit	Source
gf	-2899.49	kJ/mol	Joback Method
hf	-3187.24	kJ/mol	Joback Method
hfus	12.08	kJ/mol	Joback Method
hvap	10.76	kJ/mol	Joback Method
log10ws	-5.30		Crippen Method
logp	4.990		Crippen Method
mcvol	136.040	ml/mol	McGowan Method
pc	1675.53	kPa	Joback Method
rinpol	344.00		NIST Webbook
tb	369.50 ± 0.50	K	NIST Webbook
tc	438.67	K	Joback Method
tf	177.02	K	Joback Method
vc	0.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	311.47	J/mol×K	328.79	Joback Method
cpg	324.31	J/mol×K	347.10	Joback Method
cpg	336.47	J/mol×K	365.42	Joback Method
cpg	347.95	J/mol×K	383.73	Joback Method
cpg	358.80	J/mol×K	402.04	Joback Method
cpg	369.02	J/mol×K	420.36	Joback Method
cpg	378.63	J/mol×K	438.67	Joback Method

Sources

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=C27213612&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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