Formic acid, heptyl ester

Other names:	Heptanol, formate
	Heptyl alcohol, formate
	Heptyl formate
	formic acid heptyl ester
	heptyl alcohol formate
	heptyl methanoate
	methanoic acid, heptyl ester
	n-Heptyl formate
	n-Heptyl methanoate
Inchi:	InChI=1S/C8H16O2/c1-2-3-4-5-6-7-10-8-9/h8H,2-7H2,1H3
InchiKey:	XEAMDSXSXYAICO-UHFFFAOYSA-N
Formula:	C8H16O2
SMILES:	CCCCCCCOC=O
Mol. weight [g/mol]:	144.21
CAS:	112-23-2

Physical Properties

Property code	Value	Unit	Source
gf	-188.04	kJ/mol	Joback Method
hf	-426.25	kJ/mol	Joback Method
hfus	19.95	kJ/mol	Joback Method
hvap	42.53	kJ/mol	Joback Method
log10ws	-2.03		Crippen Method
logp	2.130		Crippen Method
mcvol	131.020	ml/mol	McGowan Method
pc	2687.42	kPa	Joback Method
rinpol	1039.00		NIST Webbook
rinpol	1039.00		NIST Webbook
rinpol	1012.00		NIST Webbook
ripol	1357.00		NIST Webbook
tb	449.90 ± 1.50	K	NIST Webbook
tb	451.27	K	KDB
tb	471.00 ± 3.00	K	NIST Webbook
tb	451.27 ± 0.30	K	NIST Webbook
tc	624.14	K	Joback Method
tf	244.15	K	Joback Method
vc	0.518	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.18	J/mol×K	624.14	Joback Method
cpg	292.78	J/mol×K	481.96	Joback Method
cpg	304.27	J/mol×K	510.39	Joback Method
cpg	315.35	J/mol×K	538.83	Joback Method
cpg	326.02	J/mol×K	567.27	Joback Method
cpg	336.30	J/mol×K	595.71	Joback Method
cpg	280.88	J/mol×K	453.52	Joback Method
dvisc	0.0037096	Pa×s	244.15	Joback Method
dvisc	0.0018311	Pa×s	279.05	Joback Method
dvisc	0.0010574	Pa×s	313.94	Joback Method
dvisc	0.0006815	Pa×s	348.83	Joback Method
dvisc	0.0004758	Pa×s	383.73	Joback Method
dvisc	0.0003527	Pa×s	418.62	Joback Method
dvisc	0.0002738	Pa×s	453.52	Joback Method
pvap	0.44	kPa	316.40	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.35	kPa	313.30	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.32	kPa	311.00	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.26	kPa	308.20	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.18	kPa	303.30	Vapour pressures and enthalpies of vaporization of aliphatic esters
pvap	0.13	kPa	298.30	Vapour pressures and enthalpies of vaporization of aliphatic esters

pvap	0.13	kPa	298.30	Vapour pressures and enthalpies of vaporization of aliphatic esters	
pvap	0.09	kPa	293.30	Vapour pressures and enthalpies of vaporization of aliphatic esters	
pvap	0.09	kPa	293.20	Vapour pressures and enthalpies of vaporization of aliphatic esters	
pvap	0.09	kPa	293.20	Vapour pressures and enthalpies of vaporization of aliphatic esters	
pvap	0.06	kPa	288.30	Vapour pressures and enthalpies of vaporization of aliphatic esters	
pvap	0.04	kPa	283.30	Vapour pressures and enthalpies of vaporization of aliphatic esters	
pvap	0.03	kPa	280.40	Vapour pressures and enthalpies of vaporization of aliphatic esters	
pvap	0.03	kPa	278.60	Vapour pressures and enthalpies of vaporization of aliphatic esters	
pvap	0.02	kPa	277.60	Vapour pressures and enthalpies of vaporization of aliphatic esters	
pvap	0.02	kPa	276.10	Vapour pressures and enthalpies of vaporization of aliphatic esters	

Correlations

Information	Value
Property code	pvap

Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54237e+01
Coeff. B	-4.15982e+03
Coeff. C	-6.62920e+01
Temperature range (K), min.	341.12
Temperature range (K), max.	477.66

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vapour pressures and enthalpies of vaporization of aliphatic esters:	https://www.doi.org/10.1016/j.fluid.2012.08.003
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1108.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C112232&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume