Heptanoyl chloride

Other names:	Enanthoyl chloride
	Enanthyl chloride
	n-Heptanoyl chloride
Inchi:	InChI=1S/C7H13ClO/c1-2-3-4-5-6-7(8)9/h2-6H2,1H3
InchiKey:	UCVODTZQZHMTPN-UHFFFAOYSA-N
Formula:	C7H13ClO
SMILES:	CCCCCCC(=O)Cl
Mol. weight [g/mol]:	148.63
CAS:	2528-61-2

Physical Properties

Property code	Value	Unit	Source
gf	-132.79	kJ/mol	Joback Method
hf	-316.13	kJ/mol	Joback Method
hfus	19.68	kJ/mol	Joback Method
hvap	42.31	kJ/mol	Joback Method
log10ws	-2.68		Crippen Method
logp	2.722		Crippen Method
mcvol	123.300	ml/mol	McGowan Method
pc	2878.12	kPa	Joback Method
rinpol	1012.10		NIST Webbook
tb	398.40	K	NIST Webbook
tb	397.00 ± 4.00	K	NIST Webbook
tb	418.00 ± 4.00	K	NIST Webbook
tb	446.20	K	NIST Webbook
tc	634.19	K	Joback Method
tf	248.50	K	Joback Method
vc	0.482	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.60	J/mol×K	634.19	Joback Method
cpg	242.45	J/mol×K	450.86	Joback Method

cpg	253.46	J/mol×K	481.42	Joback Method
cpg	263.99	J/mol×K	511.97	Joback Method
cpg	274.05	J/mol×K	542.53	Joback Method
cpg	283.67	J/mol×K	573.08	Joback Method
cpg	292.85	J/mol×K	603.64	Joback Method
dvisc	0.0003348	Pa×s	450.86	Joback Method
dvisc	0.0041001	Pa×s	248.50	Joback Method
dvisc	0.0021043	Pa×s	282.23	Joback Method
dvisc	0.0012453	Pa×s	315.95	Joback Method
dvisc	0.0008154	Pa×s	349.68	Joback Method
dvisc	0.0005752	Pa×s	383.41	Joback Method
dvisc	0.0004293	Pa×s	417.13	Joback Method
hvapt	63.70	kJ/mol	362.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.29439e+01
Coeff. B	-1.34400e+04
Coeff. C	2.56668e+02
Temperature range (K), min.	336.55
Temperature range (K), max.	505.57

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2528612&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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

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
hvapt:	Enthalpy of vaporization at a given temperature
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume