4-Propylcyclohexanone

Other names: Cyclohexanone, 4-propyl-
Inchi: InChI=1S/C9H16O/c1-2-3-8-4-6-9(10)7-5-8/h8H,2-7H2,1H3
InchiKey: NQEDLIZOPMNZMC-UHFFFAOYSA-N
Formula: C9H16O
SMILES: CCCC1CCC(=O)CC1
Mol. weight [g/mol]: 140.22
CAS: 40649-36-3

Physical Properties

Property code	Value	Unit	Source
gf	-73.24	kJ/mol	Joback Method
hf	-312.47	kJ/mol	Joback Method
hfus	10.41	kJ/mol	Joback Method
hvap	40.30	kJ/mol	Joback Method
log10ws	-2.52		Crippen Method
logp	2.546		Crippen Method
mcvol	128.380	ml/mol	McGowan Method
pc	2947.28	kPa	Joback Method
tb	492.69	K	Joback Method
tc	709.61	K	Joback Method
tf	266.79	K	Joback Method
vc	0.479	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	291.50	J/mol×K	492.69	Joback Method
cpg	309.49	J/mol×K	528.84	Joback Method
cpg	326.65	J/mol×K	565.00	Joback Method
cpg	342.98	J/mol×K	601.15	Joback Method
cpg	358.49	J/mol×K	637.31	Joback Method
cpg	373.17	J/mol×K	673.46	Joback Method
cpg	387.02	J/mol×K	709.61	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	370.70	K	2.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.60147e+01
Coeff. B	-4.48569e+03
Coeff. C	-7.63000e+01
Temperature range (K), min.	361.52
Temperature range (K), max.	495.40

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C40649363&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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume