Benzene, 1-chloro-4-propyl-

Other names: p-Chloropropylbenzene
Inchi: InChI=1S/C9H11Cl/c1-2-3-8-4-6-9(10)7-5-8/h4-7H,2-3H2,1H3
InchiKey: QXQAPNSHUJORMC-UHFFFAOYSA-N
Formula: C9H11Cl
SMILES: CCCc1ccc(Cl)cc1
Mol. weight [g/mol]: 154.64
CAS: 52944-34-0

Physical Properties

Property code	Value	Unit	Source
gf	115.75	kJ/mol	Joback Method
hf	-19.77	kJ/mol	Joback Method
hfus	16.92	kJ/mol	Joback Method
hvap	42.95	kJ/mol	Joback Method
log10ws	-3.38		Crippen Method
logp	3.292		Crippen Method
mcvol	126.150	ml/mol	McGowan Method
pc	3076.16	kPa	Joback Method
rinpol	1211.00		NIST Webbook
rinpol	1111.00		NIST Webbook
ripol	1532.00		NIST Webbook
tb	474.41	K	Joback Method
tc	689.41	K	Joback Method
tf	260.05	K	Joback Method
vc	0.480	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	242.90	J/mol×K	474.41	Joback Method
cpg	300.36	J/mol×K	653.58	Joback Method
cpg	290.24	J/mol×K	617.74	Joback Method
cpg	279.46	J/mol×K	581.91	Joback Method
cpg	267.99	J/mol×K	546.08	Joback Method

cpg	255.82	J/mol×K	510.24	Joback Method
cpg	309.86	J/mol×K	689.41	Joback Method
dvisc	0.0002456	Pa×s	474.41	Joback Method
dvisc	0.0003076	Pa×s	438.68	Joback Method
dvisc	0.0004010	Pa×s	402.96	Joback Method
dvisc	0.0005504	Pa×s	367.23	Joback Method
dvisc	0.0008087	Pa×s	331.50	Joback Method
dvisc	0.0013040	Pa×s	295.78	Joback Method
dvisc	0.0023979	Pa×s	260.05	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=C52944340&Units=SI

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
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

Latest version available from: