7-Phenyl-1-heptyl chloride

Other names: 1-Chloro-7-phenylheptane
Inchi: InChI=1S/C13H19Cl/c14-12-8-3-1-2-5-9-13-10-6-4-7-11-13/h4,6-7,10-11H,1-3,5,8-9,12H
InchiKey: PNUBJDFTMKBZJK-UHFFFAOYSA-N
Formula: C13H19Cl
SMILES: ClCCCCCCCc1ccccc1
Mol. weight [g/mol]: 210.74
CAS: 71434-47-4

Physical Properties

Property code	Value	Unit	Source
gf	159.06	kJ/mol	Joback Method
hf	-90.86	kJ/mol	Joback Method
hfus	27.66	kJ/mol	Joback Method
hvap	51.19	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	4.418		Crippen Method
mcvol	182.510	ml/mol	McGowan Method
pc	2119.73	kPa	Joback Method
tb	560.95	K	Joback Method
tc	762.24	K	Joback Method
tf	292.61	K	Joback Method
vc	0.705	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	424.66	J/mol×K	560.95	Joback Method
cpg	498.82	J/mol×K	728.69	Joback Method
cpg	485.70	J/mol×K	695.14	Joback Method
cpg	471.77	J/mol×K	661.60	Joback Method
cpg	456.98	J/mol×K	628.05	Joback Method
cpg	441.29	J/mol×K	594.50	Joback Method
cpg	511.15	J/mol×K	762.24	Joback Method
dvisc	0.0001924	Pa×s	560.95	Joback Method

dvisc	0.0002517	Pa×s	516.23	Joback Method
dvisc	0.0003465	Pa×s	471.50	Joback Method
dvisc	0.0005100	Pa×s	426.78	Joback Method
dvisc	0.0008218	Pa×s	382.06	Joback Method
dvisc	0.0015028	Pa×s	337.33	Joback Method
dvisc	0.0033048	Pa×s	292.61	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=C71434474&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume