1-Chloro-8-phenyloctane

Other names: 1-Chloro-8-phenyloctane
Inchi: InChI=1S/C14H21Cl/c15-13-9-4-2-1-3-6-10-14-11-7-5-8-12-14/h5,7-8,11-12H,1-4,6,9-10,
InchiKey: GVDYDOFBAKCSGC-UHFFFAOYSA-N
Formula: C14H21Cl
SMILES: ClCCCCCCCCc1ccccc1
Mol. weight [g/mol]: 224.78

Physical Properties

Property code	Value	Unit	Source
af	0.6306		Cheméo Relay (1.0)
gf	167.48	kJ/mol	Joback Method
hf	-117.06	kJ/mol	Cheméo Relay (1.0)
hfus	30.25	kJ/mol	Joback Method
hvap	80.91	kJ/mol	Cheméo Relay (1.0)
ie	9.20	eV	Cheméo Relay (1.0)
log10ws	-5.79		Cheméo Relay (1.0)
logp	4.809		Crippen Method
mcvol	196.600	ml/mol	McGowan Method
pc	1944.08	kPa	Joback Method
tb	566.99	K	Cheméo Relay (1.0)
tc	777.85	K	Cheméo Relay (1.0)
tf	266.12	K	Cheméo Relay (1.0)
vc	0.742	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	474.48	J/mol×K	583.83	Joback Method
cpg	563.98	J/mol×K	782.28	Joback Method
cpg	551.18	J/mol×K	749.21	Joback Method
cpg	537.60	J/mol×K	716.13	Joback Method
cpg	523.17	J/mol×K	683.06	Joback Method
cpg	507.87	J/mol×K	649.98	Joback Method
cpg	491.66	J/mol×K	616.91	Joback Method

dvisc	0.0004712	Pa×s	443.85	Joback Method
dvisc	0.0001750	Pa×s	583.83	Joback Method
dvisc	0.0002299	Pa×s	537.17	Joback Method
dvisc	0.0003181	Pa×s	490.51	Joback Method
dvisc	0.0031589	Pa×s	303.88	Joback Method
dvisc	0.0007655	Pa×s	397.20	Joback Method
dvisc	0.0014150	Pa×s	350.54	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C61440322&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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

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