4-Chlorobenzoic acid, heptyl ester

Other names: Benzoic acid, 4-chloro, heptyl ester
Heptyl 4-chlorobenzoate
Inchi: InChI=1S/C14H19ClO2/c1-2-3-4-5-6-11-17-14(16)12-7-9-13(15)10-8-12/h7-10H,2-6,11H
InchiKey: ZGRCQXNQOQBZGF-UHFFFAOYSA-N
Formula: C14H19ClO2
SMILES: CCCCCCCOC(=O)c1ccc(Cl)cc1
Mol. weight [g/mol]: 254.75
CAS: 97222-05-4

Physical Properties

Property code	Value	Unit	Source
gf	-76.07	kJ/mol	Joback Method
hf	-367.77	kJ/mol	Joback Method
hfus	32.65	kJ/mol	Joback Method
hvap	63.24	kJ/mol	Joback Method
log10ws	-4.91		Crippen Method
logp	4.467		Crippen Method
mcvol	204.040	ml/mol	McGowan Method
pc	1998.33	kPa	Joback Method
rinpol	1825.00		NIST Webbook
rinpol	1825.00		NIST Webbook
rinpol	1835.00		NIST Webbook
rinpol	1838.00		NIST Webbook
rinpol	1817.00		NIST Webbook
rinpol	1828.00		NIST Webbook
rinpol	1825.00		NIST Webbook
rinpol	1838.00		NIST Webbook
rinpol	1815.00		NIST Webbook
ripol	2372.00		NIST Webbook
ripol	2358.00		NIST Webbook
ripol	2369.00		NIST Webbook
ripol	2356.00		NIST Webbook
ripol	2369.00		NIST Webbook
ripol	2394.00		NIST Webbook
ripol	2372.00		NIST Webbook
ripol	2338.00		NIST Webbook
ripol	2369.00		NIST Webbook

tb	665.10	K	Joback Method
tc	869.77	K	Joback Method
tf	388.56	K	Joback Method
vc	0.784	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	522.84	J/mol×K	665.10	Joback Method
cpg	537.98	J/mol×K	699.21	Joback Method
cpg	552.23	J/mol×K	733.32	Joback Method
cpg	565.61	J/mol×K	767.43	Joback Method
cpg	578.16	J/mol×K	801.55	Joback Method
cpg	589.90	J/mol×K	835.66	Joback Method
cpg	600.85	J/mol×K	869.77	Joback Method
dvisc	0.0013958	Pa×s	388.56	Joback Method
dvisc	0.0007761	Pa×s	434.65	Joback Method
dvisc	0.0004830	Pa×s	480.74	Joback Method
dvisc	0.0003266	Pa×s	526.83	Joback Method
dvisc	0.0002352	Pa×s	572.92	Joback Method
dvisc	0.0001778	Pa×s	619.01	Joback Method
dvisc	0.0001398	Pa×s	665.10	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C97222054&Units=SI
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
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