Heptyl 3-chlorobenzoate

Other names: Benzoic acid, 3-chloro, heptyl ester
Inchi: InChI=1S/C14H19ClO2/c1-2-3-4-5-6-10-17-14(16)12-8-7-9-13(15)11-12/h7-9,11H,2-6,10
InchiKey: BJVCNNYBXULVBS-UHFFFAOYSA-N
Formula: C14H19ClO2
SMILES: CCCCCCCOC(=O)c1cccc(Cl)c1
Mol. weight [g/mol]: 254.75

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	1822.00		NIST Webbook
rinpol	1812.00		NIST Webbook
rinpol	1822.00		NIST Webbook
rinpol	1831.00		NIST Webbook
rinpol	1862.00		NIST Webbook
rinpol	1834.00		NIST Webbook
rinpol	1814.00		NIST Webbook
rinpol	1822.00		NIST Webbook
rinpol	1862.00		NIST Webbook
rinpol	1827.00		NIST Webbook
ripol	2370.00		NIST Webbook
ripol	2365.00		NIST Webbook
ripol	2365.00		NIST Webbook
ripol	2354.00		NIST Webbook
ripol	2365.00		NIST Webbook
ripol	2392.00		NIST Webbook
ripol	2370.00		NIST Webbook
ripol	2334.00		NIST Webbook
ripol	2353.00		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	589.90	J/mol×K	835.66	Joback Method
cpg	578.16	J/mol×K	801.55	Joback Method
cpg	565.61	J/mol×K	767.43	Joback Method
cpg	552.23	J/mol×K	733.32	Joback Method
cpg	537.98	J/mol×K	699.21	Joback Method
cpg	600.85	J/mol×K	869.77	Joback Method
dvisc	0.0001398	Pa×s	665.10	Joback Method
dvisc	0.0001778	Pa×s	619.01	Joback Method
dvisc	0.0002352	Pa×s	572.92	Joback Method
dvisc	0.0003266	Pa×s	526.83	Joback Method
dvisc	0.0004830	Pa×s	480.74	Joback Method
dvisc	0.0007761	Pa×s	434.65	Joback Method
dvisc	0.0013958	Pa×s	388.56	Joback Method

Sources

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=U373559&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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