5-Chloropentyl benzoate

Inchi: InChI=1S/C12H15ClO2/c13-9-5-2-6-10-15-12(14)11-7-3-1-4-8-11/h1,3-4,7-8H,2,5-6,9-10
InchiKey: XIOZPPYPTAEPGJ-UHFFFAOYSA-N
Formula: C12H15ClO2
SMILES: O=C(OCCCCCCl)c1ccccc1
Mol. weight [g/mol]: 226.70
CAS: 55092-47-2

Physical Properties

Property code	Value	Unit	Source
gf	-83.28	kJ/mol	Joback Method
hf	-315.02	kJ/mol	Joback Method
hfus	27.86	kJ/mol	Joback Method
hvap	58.12	kJ/mol	Joback Method
log10ws	-3.54		Crippen Method
logp	3.252		Crippen Method
mcvol	175.860	ml/mol	McGowan Method
pc	2426.65	kPa	Joback Method
tb	614.36	K	Joback Method
tc	824.31	K	Joback Method
tf	353.50	K	Joback Method
vc	0.672	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	421.99	J/mol×K	614.36	Joback Method
cpg	436.22	J/mol×K	649.35	Joback Method
cpg	449.60	J/mol×K	684.34	Joback Method
cpg	462.14	J/mol×K	719.33	Joback Method
cpg	473.87	J/mol×K	754.33	Joback Method
cpg	484.82	J/mol×K	789.32	Joback Method
cpg	495.01	J/mol×K	824.31	Joback Method
dvisc	0.0019777	Pa×s	353.50	Joback Method
dvisc	0.0010599	Pa×s	396.98	Joback Method

dvisc	0.0006425	Pa×s	440.45	Joback Method
dvisc	0.0004261	Pa×s	483.93	Joback Method
dvisc	0.0003024	Pa×s	527.41	Joback Method
dvisc	0.0002261	Pa×s	570.88	Joback Method
dvisc	0.0001762	Pa×s	614.36	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	412.50 ± 1.50	K	0.20	NIST Webbook

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=C55092472&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
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume