

5-Chlorovaleric acid, heptyl ester

Inchi:	InChI=1S/C12H23ClO2/c1-2-3-4-5-8-11-15-12(14)9-6-7-10-13/h2-11H2,1H3
InchiKey:	PSTOZFWGSOOMNV-UHFFFAOYSA-N
Formula:	C12H23ClO2
SMILES:	CCCCCCCOC(=O)CCCCCI
Mol. weight [g/mol]:	234.76
CAS:	2323-67-3

Physical Properties

Property code	Value	Unit	Source
gf	-195.69	kJ/mol	Joback Method
hf	-551.55	kJ/mol	Joback Method
hfus	33.82	kJ/mol	Joback Method
hvap	55.85	kJ/mol	Joback Method
log10ws	-3.86		Crippen Method
logp	3.909		Crippen Method
mvol	199.620	ml/mol	McGowan Method
pc	1793.94	kPa	Joback Method
rinpol	1643.90		NIST Webbook
rinpol	1643.90		NIST Webbook
tb	587.68	K	Joback Method
tc	762.26	K	Joback Method
tf	327.08	K	Joback Method
vc	0.780	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	496.42	J/mol×K	587.68	Joback Method
cpg	565.36	J/mol×K	733.17	Joback Method
cpg	552.80	J/mol×K	704.07	Joback Method
cpg	539.64	J/mol×K	674.97	Joback Method
cpg	525.87	J/mol×K	645.87	Joback Method
cpg	511.47	J/mol×K	616.78	Joback Method
cpg	577.32	J/mol×K	762.26	Joback Method

dvisc	0.0001781	Paxs	587.68	Joback Method
dvisc	0.0002330	Paxs	544.25	Joback Method
dvisc	0.0003194	Paxs	500.81	Joback Method
dvisc	0.0004650	Paxs	457.38	Joback Method
dvisc	0.0007323	Paxs	413.95	Joback Method
dvisc	0.0012830	Paxs	370.51	Joback Method
dvisc	0.0026085	Paxs	327.08	Joback Method

Sources

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=C2323673&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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
mvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/23-315-6/5-Chlorovaleric-acid-heptyl-ester.pdf>

Generated by Cheméo on 2024-04-27 02:03:53.099540823 +0000 UTC m=+16472682.020118138.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.