

5-Chlorovaleric acid, 2-naphthyl ester

Inchi:	InChI=1S/C15H15ClO2/c16-10-4-3-7-15(17)18-14-9-8-12-5-1-2-6-13(12)11-14/h1-2,5-6,8
InchiKey:	ZCUGJMUORSUDHD-UHFFFAOYSA-N
Formula:	C15H15ClO2
SMILES:	O=C(CCCCCl)Oc1ccc2ccccc2c1
Mol. weight [g/mol]:	262.73

Physical Properties

Property code	Value	Unit	Source
gf	39.00	kJ/mol	Joback Method
hf	-197.34	kJ/mol	Joback Method
hfus	32.26	kJ/mol	Joback Method
hvap	67.10	kJ/mol	Joback Method
log10ws	-5.00		Crippen Method
logp	4.154		Crippen Method
mcvol	198.670	ml/mol	McGowan Method
pc	2293.71	kPa	Joback Method
rinqol	2175.00		NIST Webbook
tb	706.96	K	Joback Method
tc	931.95	K	Joback Method
tf	432.53	K	Joback Method
vc	0.762	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	510.81	J/molxK	706.96	Joback Method
cpg	571.24	J/molxK	894.45	Joback Method
cpg	560.87	J/molxK	856.95	Joback Method
cpg	549.71	J/molxK	819.46	Joback Method
cpg	537.69	J/molxK	781.96	Joback Method
cpg	524.74	J/molxK	744.46	Joback Method
cpg	580.86	J/molxK	931.95	Joback Method
dvisc	0.0002247	Paxs	706.96	Joback Method
dvisc	0.0002719	Paxs	661.22	Joback Method

dvisc	0.0003384	Paxs	615.48	Joback Method
dvisc	0.0004362	Paxs	569.75	Joback Method
dvisc	0.0005878	Paxs	524.01	Joback Method
dvisc	0.0008386	Paxs	478.27	Joback Method
dvisc	0.0012897	Paxs	432.53	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=U307981&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
mcvol:	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

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