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
rinpol	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	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	510.81	J/mol×K	706.96	Joback Method
cpg	524.74	J/mol×K	744.46	Joback Method
cpg	537.69	J/mol×K	781.96	Joback Method
cpg	549.71	J/mol×K	819.46	Joback Method
cpg	560.87	J/mol×K	856.95	Joback Method
cpg	571.24	J/mol×K	894.45	Joback Method
cpg	580.86	J/mol×K	931.95	Joback Method
dvisc	0.0012897	Pa×s	432.53	Joback Method
dvisc	0.0008386	Pa×s	478.27	Joback Method

dvisc	0.0005878	Pa×s	524.01	Joback Method
dvisc	0.0004362	Pa×s	569.75	Joback Method
dvisc	0.0003384	Pa×s	615.48	Joback Method
dvisc	0.0002719	Pa×s	661.22	Joback Method
dvisc	0.0002247	Pa×s	706.96	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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