5-chlorovaleric acid, undecyl ester

Inchi: InChI=1S/C16H31ClO2/c1-2-3-4-5-6-7-8-9-12-15-19-16(18)13-10-11-14-17/h2-15H2,1H3
InchiKey: MZLDFDLDFGBNEV-UHFFFAOYSA-N
Formula: C16H31ClO2
SMILES: CCCCCCCCCCCOC(=O)CCCCCl
Mol. weight [g/mol]: 290.87

Physical Properties

Property code	Value	Unit	Source
af	0.8723		Cheméo Relay (1.0)
hf	-724.00	kJ/mol	Cheméo Relay (1.0)
hfus	44.18	kJ/mol	Joback Method
hvap	88.23	kJ/mol	Cheméo Relay (1.0)
ie	9.88	eV	Cheméo Relay (1.0)
log10ws	-5.64		Cheméo Relay (1.0)
logp	5.470		Crippen Method
mcvol	255.980	ml/mol	McGowan Method
pc	1327.14	kPa	Joback Method
rinpol	2064.10		NIST Webbook
tb	581.11	K	Cheméo Relay (1.0)
tc	771.36	K	Cheméo Relay (1.0)
tf	278.10	K	Cheméo Relay (1.0)
vc	0.977	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	710.59	J/mol×K	679.20	Joback Method
cpg	727.71	J/mol×K	707.92	Joback Method
cpg	744.05	J/mol×K	736.64	Joback Method
cpg	759.63	J/mol×K	765.36	Joback Method
cpg	774.47	J/mol×K	794.09	Joback Method
cpg	788.57	J/mol×K	822.81	Joback Method
cpg	801.97	J/mol×K	851.53	Joback Method
dvisc	0.0019268	Pa×s	372.16	Joback Method

dvisc	0.0008962	Pa×s	423.33	Joback Method
dvisc	0.0004917	Pa×s	474.51	Joback Method
dvisc	0.0003032	Pa×s	525.68	Joback Method
dvisc	0.0002037	Pa×s	576.85	Joback Method
dvisc	0.0001460	Pa×s	628.03	Joback Method
dvisc	0.0001101	Pa×s	679.20	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C52893206&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
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