6-Chlorohexanoic acid, 2-naphthyl ester

Inchi: InChI=1S/C16H17ClO2/c17-11-5-1-2-8-16(18)19-15-10-9-13-6-3-4-7-14(13)12-15/h3-4,6
InchiKey: BPYZYGDDNGIIMV-UHFFFAOYSA-N
Formula: C16H17ClO2
SMILES: O=C(CCCCCCl)Oc1ccc2ccccc2c1
Mol. weight [g/mol]: 276.76

Physical Properties

Property code	Value	Unit	Source
gf	47.42	kJ/mol	Joback Method
hf	-217.98	kJ/mol	Joback Method
hfus	34.85	kJ/mol	Joback Method
hvap	69.33	kJ/mol	Joback Method
log10ws	-5.42		Crippen Method
logp	4.544		Crippen Method
mcvol	212.760	ml/mol	McGowan Method
pc	2096.50	kPa	Joback Method
rinpol	2302.00		NIST Webbook
tb	729.84	K	Joback Method
tc	951.12	K	Joback Method
tf	443.80	K	Joback Method
vc	0.819	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	563.50	J/mol×K	729.84	Joback Method
cpg	577.86	J/mol×K	766.72	Joback Method
cpg	591.22	J/mol×K	803.60	Joback Method
cpg	603.65	J/mol×K	840.48	Joback Method
cpg	615.21	J/mol×K	877.36	Joback Method
cpg	625.97	J/mol×K	914.24	Joback Method
cpg	635.99	J/mol×K	951.12	Joback Method
dvisc	0.0012279	Pa×s	443.80	Joback Method
dvisc	0.0007860	Pa×s	491.47	Joback Method

dvisc	0.0005444	Pa×s	539.15	Joback Method
dvisc	0.0004002	Pa×s	586.82	Joback Method
dvisc	0.0003082	Pa×s	634.49	Joback Method
dvisc	0.0002461	Pa×s	682.17	Joback Method
dvisc	0.0002024	Pa×s	729.84	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U307626&Units=SI

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