3-Cyclopentylpropionic acid, 8-chlorooctyl ester

Inchi: InChI=1S/C16H29ClO2/c17-13-7-3-1-2-4-8-14-19-16(18)12-11-15-9-5-6-10-15/h15H,1-14

InchiKey: LSPFYISYDAUGPA-UHFFFAOYSA-N

Formula: C16H29ClO2

SMILES: O=C(CCC1CCCC1)OCCCCCCCCCl

Mol. weight [g/mol]: 288.85

Physical Properties

Property code	Value	Unit	Source
gf	-125.46	kJ/mol	Joback Method
hf	-573.63	kJ/mol	Joback Method
hfus	38.12	kJ/mol	Joback Method
hvap	65.01	kJ/mol	Joback Method
log10ws	-5.19		Crippen Method
logp	5.079		Crippen Method
mcvol	245.120	ml/mol	McGowan Method
pc	1519.94	kPa	Joback Method
rinpol	2198.00		NIST Webbook
rinpol	2198.00		NIST Webbook
tb	694.48	K	Joback Method
tc	883.75	K	Joback Method
tf	383.06	K	Joback Method
vc	0.946	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	702.55	J/mol×K	694.48	Joback Method
cpg	721.18	J/mol×K	726.03	Joback Method
cpg	738.81	J/mol×K	757.57	Joback Method
cpg	755.46	J/mol×K	789.12	Joback Method
cpg	771.15	J/mol×K	820.66	Joback Method
cpg	785.93	J/mol×K	852.21	Joback Method
cpg	799.83	J/mol×K	883.75	Joback Method
dvisc	0.0022482	Pa×s	383.06	Joback Method

dvisc	0.0011094	Pa×s	434.96	Joback Method
dvisc	0.0006364	Pa×s	486.87	Joback Method
dvisc	0.0004063	Pa×s	538.77	Joback Method
dvisc	0.0002807	Pa×s	590.67	Joback Method
dvisc	0.0002059	Pa×s	642.58	Joback Method
dvisc	0.0001581	Pa×s	694.48	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=U354058&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