3-Cyclopentylpropionic acid, undecyl ester

Inchi: InChI=1S/C19H36O2/c1-2-3-4-5-6-7-8-9-12-17-21-19(20)16-15-18-13-10-11-14-18/h18H
InchiKey: PCABZFXNXVVEDP-UHFFFAOYSA-N
Formula: C19H36O2
SMILES: CCCCCCCCCCCOC(=O)CCC1CCCC1
Mol. weight [g/mol]: 296.49

Physical Properties

Property code	Value	Unit	Source
gf	-88.27	kJ/mol	Joback Method
hf	-619.81	kJ/mol	Joback Method
hfus	41.69	kJ/mol	Joback Method
hvap	67.30	kJ/mol	Joback Method
log10ws	-6.29		Crippen Method
logp	6.031		Crippen Method
mcvol	275.150	ml/mol	McGowan Method
pc	1261.06	kPa	Joback Method
rinpol	2165.90		NIST Webbook
tb	725.69	K	Joback Method
tc	908.60	K	Joback Method
tf	386.95	K	Joback Method
vc	1.065	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	842.28	J/mol×K	725.69	Joback Method
cpg	934.07	J/mol×K	878.12	Joback Method
cpg	917.72	J/mol×K	847.63	Joback Method
cpg	900.40	J/mol×K	817.15	Joback Method
cpg	882.07	J/mol×K	786.66	Joback Method
cpg	862.71	J/mol×K	756.18	Joback Method
cpg	949.48	J/mol×K	908.60	Joback Method
dvisc	0.0001214	Pa×s	725.69	Joback Method
dvisc	0.0001601	Pa×s	669.23	Joback Method

dvisc	0.0002221	Pa×s	612.78	Joback Method
dvisc	0.0003294	Pa×s	556.32	Joback Method
dvisc	0.0005339	Pa×s	499.86	Joback Method
dvisc	0.0009785	Pa×s	443.41	Joback Method
dvisc	0.0021404	Pa×s	386.95	Joback Method

Sources

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=U292271&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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