3-Cyclopentylpropionic acid, heptyl ester

Inchi: InChI=1S/C15H28O2/c1-2-3-4-5-8-13-17-15(16)12-11-14-9-6-7-10-14/h14H,2-13H2,1H3
InchiKey: OBXCQEYVYLJGJK-UHFFFAOYSA-N
Formula: C15H28O2
SMILES: CCCCCCCOC(=O)CCC1CCCC1
Mol. weight [g/mol]: 240.38

Physical Properties

Property code	Value	Unit	Source
gf	-121.95	kJ/mol	Joback Method
hf	-537.25	kJ/mol	Joback Method
hfus	31.33	kJ/mol	Joback Method
hvap	58.40	kJ/mol	Joback Method
log10ws	-4.62		Crippen Method
logp	4.470		Crippen Method
mcvol	218.790	ml/mol	McGowan Method
pc	1690.72	kPa	Joback Method
rinpol	1754.80		NIST Webbook
tb	634.17	K	Joback Method
tc	820.80	K	Joback Method
tf	341.87	K	Joback Method
vc	0.841	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	612.21	J/mol×K	634.17	Joback Method
cpg	699.75	J/mol×K	789.70	Joback Method
cpg	684.09	J/mol×K	758.59	Joback Method
cpg	667.54	J/mol×K	727.49	Joback Method
cpg	650.05	J/mol×K	696.38	Joback Method
cpg	631.62	J/mol×K	665.28	Joback Method
cpg	714.54	J/mol×K	820.80	Joback Method
dvisc	0.0001934	Pa×s	634.17	Joback Method
dvisc	0.0002515	Pa×s	585.45	Joback Method

dvisc	0.0003430	Pa×s	536.74	Joback Method
dvisc	0.0004977	Pa×s	488.02	Joback Method
dvisc	0.0007845	Pa×s	439.30	Joback Method
dvisc	0.0013850	Pa×s	390.59	Joback Method
dvisc	0.0028751	Pa×s	341.87	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=U292333&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