

3-Cyclopentylpropionic acid, decyl ester

Inchi: InChI=1S/C18H34O2/c1-2-3-4-5-6-7-8-11-16-20-18(19)15-14-17-12-9-10-13-17/h17H,2-1
InchiKey: VNQAHVRLXYNRKW-UHFFFAOYSA-N
Formula: C18H34O2
SMILES: CCCCCCCCCCOC(=O)CCC1CCCC1
Mol. weight [g/mol]: 282.46

Physical Properties

Property code	Value	Unit	Source
gf	-96.69	kJ/mol	Joback Method
hf	-599.17	kJ/mol	Joback Method
hfus	39.10	kJ/mol	Joback Method
hvap	65.08	kJ/mol	Joback Method
log10ws	-5.87		Crippen Method
logp	5.641		Crippen Method
mcvol	261.060	ml/mol	McGowan Method
pc	1351.64	kPa	Joback Method
rinpol	2048.20		NIST Webbook
tb	702.81	K	Joback Method
tc	885.99	K	Joback Method
tf	375.68	K	Joback Method
vc	1.008	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	783.10	J/mol×K	702.81	Joback Method
cpg	803.31	J/mol×K	733.34	Joback Method
cpg	822.47	J/mol×K	763.87	Joback Method
cpg	840.63	J/mol×K	794.40	Joback Method
cpg	857.80	J/mol×K	824.93	Joback Method
cpg	874.01	J/mol×K	855.46	Joback Method
cpg	889.31	J/mol×K	885.99	Joback Method
dvisc	0.0023287	Pa×s	375.68	Joback Method
dvisc	0.0010775	Pa×s	430.20	Joback Method

dvisc	0.0005929	Pa×s	484.72	Joback Method
dvisc	0.0003682	Pa×s	539.25	Joback Method
dvisc	0.0002495	Pa×s	593.77	Joback Method
dvisc	0.0001805	Pa×s	648.29	Joback Method
dvisc	0.0001374	Pa×s	702.81	Joback Method

Sources

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=U292336&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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