

3-Cyclopentylpropionic acid, hexyl ester

Inchi:	InChI=1S/C14H26O2/c1-2-3-4-7-12-16-14(15)11-10-13-8-5-6-9-13/h13H,2-12H2,1H3
InchiKey:	KGSNANUYCZAHJK-UHFFFAOYSA-N
Formula:	C14H26O2
SMILES:	CCCCCOC(=O)CCC1CCCC1
Mol. weight [g/mol]:	226.35

Physical Properties

Property code	Value	Unit	Source
gf	-130.37	kJ/mol	Joback Method
hf	-516.61	kJ/mol	Joback Method
hfus	28.74	kJ/mol	Joback Method
hvap	56.17	kJ/mol	Joback Method
log10ws	-4.20		Crippen Method
logp	4.080		Crippen Method
mcvol	204.700	ml/mol	McGowan Method
pc	1832.54	kPa	Joback Method
rinpol	1664.80		NIST Webbook
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tb	611.29	K	Joback Method
tc	799.78	K	Joback Method
tf	330.60	K	Joback Method
vc	0.784	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	557.74	J/molxK	611.29	Joback Method
cpg	643.74	J/molxK	768.37	Joback Method
cpg	628.35	J/molxK	736.95	Joback Method
cpg	612.08	J/molxK	705.54	Joback Method
cpg	594.90	J/molxK	674.12	Joback Method
cpg	576.80	J/molxK	642.71	Joback Method
cpg	658.28	J/molxK	799.78	Joback Method
dvisc	0.0002144	Paxs	611.29	Joback Method

dvisc	0.0002776	Paxs	564.51	Joback Method
dvisc	0.0003768	Paxs	517.73	Joback Method
dvisc	0.0005434	Paxs	470.94	Joback Method
dvisc	0.0008494	Paxs	424.16	Joback Method
dvisc	0.0014835	Paxs	377.38	Joback Method
dvisc	0.0030337	Paxs	330.60	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292334&Units=SI
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

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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