

3-Cyclopentylpropionic acid, 2-methylpentyl ester

Inchi:	InChI=1S/C14H26O2/c1-3-6-12(2)11-16-14(15)10-9-13-7-4-5-8-13/h12-13H,3-11H2,1-2H
InchiKey:	MGFKGBKGQDWMB5-UHFFFAOYSA-N
Formula:	C14H26O2
SMILES:	CCCC(C)COC(=O)CCC1CCCC1
Mol. weight [g/mol]:	226.35

Physical Properties

Property code	Value	Unit	Source
gf	-132.81	kJ/mol	Joback Method
hf	-521.89	kJ/mol	Joback Method
hfus	25.21	kJ/mol	Joback Method
hvap	55.78	kJ/mol	Joback Method
log10ws	-3.96		Crippen Method
logp	3.936		Crippen Method
mcvol	204.700	ml/mol	McGowan Method
pc	1845.16	kPa	Joback Method
rinqol	1620.00		NIST Webbook
tb	610.85	K	Joback Method
tc	802.78	K	Joback Method
tf	315.60	K	Joback Method
vc	0.778	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.10	J/molxK	610.85	Joback Method
cpg	645.64	J/molxK	770.79	Joback Method
cpg	630.02	J/molxK	738.80	Joback Method
cpg	613.49	J/molxK	706.81	Joback Method
cpg	596.00	J/molxK	674.83	Joback Method
cpg	577.55	J/molxK	642.84	Joback Method
cpg	660.37	J/molxK	802.78	Joback Method
dvisc	0.0001999	Paxs	610.85	Joback Method
dvisc	0.0002643	Paxs	561.64	Joback Method

dvisc	0.0003686	Paxs	512.43	Joback Method
dvisc	0.0005517	Paxs	463.23	Joback Method
dvisc	0.0009088	Paxs	414.02	Joback Method
dvisc	0.0017131	Paxs	364.81	Joback Method
dvisc	0.0039350	Paxs	315.60	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354330&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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