

3-Cyclopentylpropionic acid, nonyl ester

Inchi:	InChI=1S/C17H32O2/c1-2-3-4-5-6-7-10-15-19-17(18)14-13-16-11-8-9-12-16/h16H,2-15H
InchiKey:	CBEWPYVMEYHIPC-UHFFFAOYSA-N
Formula:	C17H32O2
SMILES:	CCCCCCCCCOC(=O)CCC1CCCC1
Mol. weight [g/mol]:	268.43

Physical Properties

Property code	Value	Unit	Source
gf	-105.11	kJ/mol	Joback Method
hf	-578.53	kJ/mol	Joback Method
hfus	36.51	kJ/mol	Joback Method
hvap	62.85	kJ/mol	Joback Method
log10ws	-5.45		Crippen Method
logp	5.251		Crippen Method
mcvol	246.970	ml/mol	McGowan Method
pc	1452.35	kPa	Joback Method
tb	679.93	K	Joback Method
tc	863.86	K	Joback Method
tf	364.41	K	Joback Method
vc	0.953	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	724.98	J/molxK	679.93	Joback Method
cpg	814.92	J/molxK	833.20	Joback Method
cpg	798.86	J/molxK	802.55	Joback Method
cpg	781.86	J/molxK	771.89	Joback Method
cpg	763.90	J/molxK	741.24	Joback Method
cpg	744.95	J/molxK	710.58	Joback Method
cpg	830.07	J/molxK	863.86	Joback Method
dvisc	0.0001547	Paxs	679.93	Joback Method
dvisc	0.0002027	Paxs	627.34	Joback Method
dvisc	0.0002790	Paxs	574.76	Joback Method

dvisc	0.0004095	Paxs	522.17	Joback Method
dvisc	0.0006550	Paxs	469.58	Joback Method
dvisc	0.0011794	Paxs	417.00	Joback Method
dvisc	0.0025169	Paxs	364.41	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292268&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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