

Pimelic acid, di(pentyl) ester

Other names:	Diamyl pimelate
Inchi:	InChI=1S/C17H32O4/c1-3-5-10-14-20-16(18)12-8-7-9-13-17(19)21-15-11-6-4-2/h3-15H2
InchiKey:	HVOBSMMTXJMTIU-UHFFFAOYSA-N
Formula:	C17H32O4
SMILES:	CCCCCOC(=O)CCCCC(=O)OCCCCC
Mol. weight [g/mol]:	300.43

Physical Properties

Property code	Value	Unit	Source
gf	-375.58	kJ/mol	Joback Method
hf	-883.81	kJ/mol	Joback Method
hfus	45.36	kJ/mol	Joback Method
hvap	71.75	kJ/mol	Joback Method
log10ws	-4.66		Crippen Method
logp	4.404		Crippen Method
mcvol	265.270	ml/mol	McGowan Method
pc	1314.65	kPa	Joback Method
rinpol	2084.00		NIST Webbook
rinpol	2019.00		NIST Webbook
rinpol	2019.00		NIST Webbook
rinpol	2084.00		NIST Webbook
tb	740.94	K	Joback Method
tc	918.14	K	Joback Method
tf	425.67	K	Joback Method
vc	1.036	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	791.03	J/molxK	740.94	Joback Method
cpg	808.03	J/molxK	770.47	Joback Method
cpg	824.15	J/molxK	800.01	Joback Method
cpg	839.43	J/molxK	829.54	Joback Method
cpg	853.86	J/molxK	859.07	Joback Method

cpg	867.46	J/mol×K	888.60	Joback Method
cpg	880.23	J/mol×K	918.14	Joback Method
dvisc	0.0011435	Paxs	425.67	Joback Method
dvisc	0.0005773	Paxs	478.21	Joback Method
dvisc	0.0003337	Paxs	530.76	Joback Method
dvisc	0.0002129	Paxs	583.31	Joback Method
dvisc	0.0001463	Paxs	635.85	Joback Method
dvisc	0.0001065	Paxs	688.39	Joback Method
dvisc	0.0000811	Paxs	740.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393824&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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