

Pimelic acid, 4-methyl-2-pentyl 3-methyl-2-pentyl ester

Inchi:	InChI=1S/C19H36O4/c1-7-15(4)17(6)23-19(21)12-10-8-9-11-18(20)22-16(5)13-14(2)3/h
InchiKey:	ZHJDDXAHACBHBF-UHFFFAOYSA-N
Formula:	C19H36O4
SMILES:	CCC(C)C(C)OC(=O)CCCCC(=O)OC(C)CC(C)C
Mol. weight [g/mol]:	328.49

Physical Properties

Property code	Value	Unit	Source
gf	-368.50	kJ/mol	Joback Method
hf	-946.21	kJ/mol	Joback Method
hfus	36.45	kJ/mol	Joback Method
hvap	74.65	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	4.893		Crippen Method
mcvol	293.450	ml/mol	McGowan Method
pc	1174.44	kPa	Joback Method
rinsol	2165.00		NIST Webbook
tb	784.94	K	Joback Method
tc	970.70	K	Joback Method
tf	388.21	K	Joback Method
vc	1.123	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	910.84	J/molxK	784.94	Joback Method
cpg	929.17	J/molxK	815.90	Joback Method
cpg	946.44	J/molxK	846.86	Joback Method
cpg	962.66	J/molxK	877.82	Joback Method
cpg	977.85	J/molxK	908.78	Joback Method
cpg	992.02	J/molxK	939.74	Joback Method
cpg	1005.19	J/molxK	970.70	Joback Method
dvisc	0.0021477	Paxs	388.21	Joback Method
dvisc	0.0007008	Paxs	454.33	Joback Method

dvisc	0.0003040	Paxs	520.45	Joback Method
dvisc	0.0001591	Paxs	586.58	Joback Method
dvisc	0.0000950	Paxs	652.70	Joback Method
dvisc	0.0000624	Paxs	718.82	Joback Method
dvisc	0.0000439	Paxs	784.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406596&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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