

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

Inchi:	InChI=1S/C18H34O4/c1-5-6-10-13-21-17(19)11-8-7-9-12-18(20)22-16(4)14-15(2)3/h15-1
InchiKey:	DDIMGLSGSNLMQK-UHFFFAOYSA-N
Formula:	C18H34O4
SMILES:	CCCCCOC(=O)CCCCC(=O)OC(C)CC(C)C
Mol. weight [g/mol]:	314.46

Physical Properties

Property code	Value	Unit	Source
gf	-372.04	kJ/mol	Joback Method
hf	-915.01	kJ/mol	Joback Method
hfus	40.90	kJ/mol	Joback Method
hvap	73.20	kJ/mol	Joback Method
log10ws	-4.95		Crippen Method
logp	4.648		Crippen Method
mvol	279.360	ml/mol	McGowan Method
pc	1241.58	kPa	Joback Method
rinpol	2034.00		NIST Webbook
rinpol	2034.00		NIST Webbook
tb	762.94	K	Joback Method
tc	944.42	K	Joback Method
tf	406.94	K	Joback Method
vc	1.079	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	850.46	J/molxK	762.94	Joback Method
cpg	868.17	J/molxK	793.19	Joback Method
cpg	884.91	J/molxK	823.43	Joback Method
cpg	900.70	J/molxK	853.68	Joback Method
cpg	915.55	J/molxK	883.93	Joback Method
cpg	929.48	J/molxK	914.17	Joback Method
cpg	942.50	J/molxK	944.42	Joback Method
dvisc	0.0015163	Paxs	406.94	Joback Method

dvisc	0.0006283	Paxs	466.27	Joback Method
dvisc	0.0003176	Paxs	525.61	Joback Method
dvisc	0.0001844	Paxs	584.94	Joback Method
dvisc	0.0001183	Paxs	644.27	Joback Method
dvisc	0.0000818	Paxs	703.61	Joback Method
dvisc	0.0000599	Paxs	762.94	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393810&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

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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