

Pimelic acid, isobutyl 2-methylpentyl ester

Inchi:	InChI=1S/C17H32O4/c1-5-9-15(4)13-21-17(19)11-8-6-7-10-16(18)20-12-14(2)3/h14-15H
InchiKey:	YZAOKOMZFUVDP-UHFFFAOYSA-N
Formula:	C17H32O4
SMILES:	CCCC(C)COC(=O)CCCCC(=O)OCC(C)C
Mol. weight [g/mol]:	300.43

Physical Properties

Property code	Value	Unit	Source
gf	-380.46	kJ/mol	Joback Method
hf	-894.37	kJ/mol	Joback Method
hfus	38.31	kJ/mol	Joback Method
hvap	70.97	kJ/mol	Joback Method
log10ws	-4.18		Crippen Method
logp	4.115		Crippen Method
mcvol	265.270	ml/mol	McGowan Method
pc	1330.04	kPa	Joback Method
rinpol	1974.00		NIST Webbook
rinpol	1974.00		NIST Webbook
tb	740.06	K	Joback Method
tc	920.59	K	Joback Method
tf	395.67	K	Joback Method
vc	1.024	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	792.00	J/molxK	740.06	Joback Method
cpg	809.35	J/molxK	770.15	Joback Method
cpg	825.78	J/molxK	800.24	Joback Method
cpg	841.31	J/molxK	830.32	Joback Method
cpg	855.95	J/molxK	860.41	Joback Method
cpg	869.70	J/molxK	890.50	Joback Method
cpg	882.59	J/molxK	920.59	Joback Method
dvisc	0.0016971	Paxs	395.67	Joback Method

dvisc	0.0007096	Paxs	453.07	Joback Method
dvisc	0.0003610	Paxs	510.47	Joback Method
dvisc	0.0002105	Paxs	567.87	Joback Method
dvisc	0.0001355	Paxs	625.26	Joback Method
dvisc	0.0000940	Paxs	682.66	Joback Method
dvisc	0.0000690	Paxs	740.06	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406663&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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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