

di-(1-Methyl-2-methoxybutyl)pimelate

Inchi:	InChI=1S/C17H32O6/c1-12(20-5)14(3)22-16(18)10-8-7-9-11-17(19)23-15(4)13(2)21-6/h
InchiKey:	UBJJGSASEAGHLB-UHFFFAOYSA-N
Formula:	C17H32O6
SMILES:	COC(C)C(C)OC(=O)CCCCCC(=O)OC(C)C(C)OC
Mol. weight [g/mol]:	332.43

Physical Properties

Property code	Value	Unit	Source
gf	-595.34	kJ/mol	Joback Method
hf	-1169.37	kJ/mol	Joback Method
hfus	33.64	kJ/mol	Joback Method
hvap	75.02	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	2.870		Crippen Method
mcvol	277.010	ml/mol	McGowan Method
pc	1312.75	kPa	Joback Method
rinpola	1888.00		NIST Webbook
rinpola	1888.00		NIST Webbook
tb	784.02	K	Joback Method
tc	970.49	K	Joback Method
tf	410.13	K	Joback Method
vc	1.048	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	854.08	J/molxK	784.02	Joback Method
cpg	871.17	J/molxK	815.10	Joback Method
cpg	887.19	J/molxK	846.18	Joback Method
cpg	902.15	J/molxK	877.26	Joback Method
cpg	916.02	J/molxK	908.34	Joback Method
cpg	928.81	J/molxK	939.41	Joback Method
cpg	940.49	J/molxK	970.49	Joback Method
dvisc	0.0011357	Paxs	410.13	Joback Method

dvisc	0.0004268	Paxs	472.44	Joback Method
dvisc	0.0002015	Paxs	534.76	Joback Method
dvisc	0.0001112	Paxs	597.08	Joback Method
dvisc	0.0000687	Paxs	659.39	Joback Method
dvisc	0.0000461	Paxs	721.70	Joback Method
dvisc	0.0000330	Paxs	784.02	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R541869&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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