

di-(3-Methoxybutyl)pimelate

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

Physical Properties

Property code	Value	Unit	Source
gf	-590.46	kJ/mol	Joback Method
hf	-1158.81	kJ/mol	Joback Method
hfus	40.69	kJ/mol	Joback Method
hvap	75.79	kJ/mol	Joback Method
log10ws	-3.06		Crippen Method
logp	2.873		Crippen Method
mvol	277.010	ml/mol	McGowan Method
pc	1297.66	kPa	Joback Method
rinpol	2139.00		NIST Webbook
rinpol	2139.00		NIST Webbook
tb	784.90	K	Joback Method
tc	968.53	K	Joback Method
tf	440.13	K	Joback Method
vc	1.060	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	853.07	J/molxK	784.90	Joback Method
cpg	869.89	J/molxK	815.50	Joback Method
cpg	885.69	J/molxK	846.11	Joback Method
cpg	900.47	J/molxK	876.71	Joback Method
cpg	914.22	J/molxK	907.32	Joback Method
cpg	926.93	J/molxK	937.92	Joback Method
cpg	938.59	J/molxK	968.53	Joback Method
dvisc	0.0007540	Paxs	440.13	Joback Method

dvisc	0.0003461	Paxs	497.59	Joback Method
dvisc	0.0001867	Paxs	555.05	Joback Method
dvisc	0.0001130	Paxs	612.51	Joback Method
dvisc	0.0000746	Paxs	669.98	Joback Method
dvisc	0.0000526	Paxs	727.44	Joback Method
dvisc	0.0000390	Paxs	784.90	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=R542253&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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