

Pimelic acid, di(5-methoxy-3-methylpent-2-yl) ester

Inchi:	InChI=1S/C21H40O6/c1-16(12-14-24-5)18(3)26-20(22)10-8-7-9-11-21(23)27-19(4)17(2)
InchiKey:	ZCJYYJAUDKDLKA-UHFFFAOYSA-N
Formula:	C21H40O6
SMILES:	COCCC(C)C(C)OC(=O)CCCCC(=O)OC(C)C(C)CCOC
Mol. weight [g/mol]:	388.54

Physical Properties

Property code	Value	Unit	Source
gf	-561.66	kJ/mol	Joback Method
hf	-1251.93	kJ/mol	Joback Method
hfus	44.00	kJ/mol	Joback Method
hvap	83.92	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	4.146		Crippen Method
mcvol	333.370	ml/mol	McGowan Method
pc	1011.66	kPa	Joback Method
rinsol	2463.00		NIST Webbook
tb	875.54	K	Joback Method
tc	1072.38	K	Joback Method
tf	455.21	K	Joback Method
vc	1.272	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1095.56	J/molxK	875.54	Joback Method
cpg	1172.21	J/molxK	1039.57	Joback Method
cpg	1159.69	J/molxK	1006.77	Joback Method
cpg	1145.76	J/molxK	973.96	Joback Method
cpg	1130.43	J/molxK	941.15	Joback Method
cpg	1113.70	J/molxK	908.35	Joback Method
cpg	1183.33	J/molxK	1072.38	Joback Method
dvisc	0.0000178	Paxs	875.54	Joback Method
dvisc	0.0000250	Paxs	805.48	Joback Method

dvisc	0.0000375	Paxs	735.43	Joback Method
dvisc	0.0000612	Paxs	665.38	Joback Method
dvisc	0.0001121	Paxs	595.32	Joback Method
dvisc	0.0002412	Paxs	525.26	Joback Method
dvisc	0.0006569	Paxs	455.21	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=U406731&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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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