

Pimelic acid, 4-methoxybenzyl propyl ester

Inchi:	InChI=1S/C18H26O5/c1-3-13-22-17(19)7-5-4-6-8-18(20)23-14-15-9-11-16(21-2)12-10-15
InchiKey:	ITUFAQYRXJONCB-UHFFFAOYSA-N
Formula:	C18H26O5
SMILES:	CCCOC(=O)CCCCC(=O)OCc1ccc(OC)cc1
Mol. weight [g/mol]:	322.40

Physical Properties

Property code	Value	Unit	Source
gf	-369.38	kJ/mol	Joback Method
hf	-811.61	kJ/mol	Joback Method
hfus	42.79	kJ/mol	Joback Method
hvap	79.32	kJ/mol	Joback Method
log10ws	-4.38		Crippen Method
logp	3.642		Crippen Method
mcvol	261.470	ml/mol	McGowan Method
pc	1531.86	kPa	Joback Method
rinpol	2470.00		NIST Webbook
rinpol	2470.00		NIST Webbook
tb	817.90	K	Joback Method
tc	1017.91	K	Joback Method
tf	498.11	K	Joback Method
vc	1.002	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	790.00	J/molxK	817.90	Joback Method
cpg	855.27	J/molxK	984.57	Joback Method
cpg	844.40	J/molxK	951.24	Joback Method
cpg	832.44	J/molxK	917.90	Joback Method
cpg	819.39	J/molxK	884.57	Joback Method
cpg	805.25	J/molxK	851.23	Joback Method
cpg	865.06	J/molxK	1017.91	Joback Method
dvisc	0.0000544	Paxs	817.90	Joback Method

dvisc	0.0000694	Paxs	764.60	Joback Method
dvisc	0.0000917	Paxs	711.30	Joback Method
dvisc	0.0001268	Paxs	658.00	Joback Method
dvisc	0.0001857	Paxs	604.71	Joback Method
dvisc	0.0002926	Paxs	551.41	Joback Method
dvisc	0.0005083	Paxs	498.11	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416536&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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