

Pimelic acid, 4-methoxybenzyl octyl ester

Inchi:	InChI=1S/C23H36O5/c1-3-4-5-6-7-11-18-27-22(24)12-9-8-10-13-23(25)28-19-20-14-16-2
InchiKey:	AGMQTAWBVLSEEA-UHFFFAOYSA-N
Formula:	C23H36O5
SMILES:	CCCCCCCCOC(=O)CCCCC(=O)OCc1ccc(OC)cc1
Mol. weight [g/mol]:	392.53

Physical Properties

Property code	Value	Unit	Source
gf	-327.28	kJ/mol	Joback Method
hf	-914.81	kJ/mol	Joback Method
hfus	55.74	kJ/mol	Joback Method
hvap	90.45	kJ/mol	Joback Method
log10ws	-6.47		Crippen Method
logp	5.593		Crippen Method
mvol	331.920	ml/mol	McGowan Method
pc	1085.63	kPa	Joback Method
rinpol	3014.00		NIST Webbook
rinpol	3014.00		NIST Webbook
tb	932.30	K	Joback Method
tc	1142.00	K	Joback Method
tf	554.46	K	Joback Method
vc	1.282	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1087.84	J/molxK	932.30	Joback Method
cpg	1154.64	J/molxK	1107.05	Joback Method
cpg	1144.07	J/molxK	1072.10	Joback Method
cpg	1132.12	J/molxK	1037.15	Joback Method
cpg	1118.78	J/molxK	1002.20	Joback Method
cpg	1104.03	J/molxK	967.25	Joback Method
cpg	1163.87	J/molxK	1142.00	Joback Method
dvisc	0.0000265	Paxs	932.30	Joback Method

dvisc	0.0000343	Paxs	869.33	Joback Method
dvisc	0.0000462	Paxs	806.35	Joback Method
dvisc	0.0000654	Paxs	743.38	Joback Method
dvisc	0.0000989	Paxs	680.41	Joback Method
dvisc	0.0001626	Paxs	617.43	Joback Method
dvisc	0.0002993	Paxs	554.46	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416543&Units=SI

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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