

p-Methoxybenzoic acid, 5-phenylpentyl ester

Inchi:	InChI=1S/C19H22O3/c1-21-18-13-11-17(12-14-18)19(20)22-15-7-3-6-10-16-8-4-2-5-9-16
InchiKey:	HHRNPMGBOAYALH-UHFFFAOYSA-N
Formula:	C19H22O3
SMILES:	COc1ccc(C(=O)OCCCCc2ccccc2)cc1
Mol. weight [g/mol]:	298.38

Physical Properties

Property code	Value	Unit	Source
gf	-14.63	kJ/mol	Joback Method
hf	-350.92	kJ/mol	Joback Method
hfus	36.63	kJ/mol	Joback Method
hvap	74.67	kJ/mol	Joback Method
log10ws	-5.12		Crippen Method
logp	4.265		Crippen Method
mcvol	244.360	ml/mol	McGowan Method
pc	1786.37	kPa	Joback Method
rinpol	2648.70		NIST Webbook
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tb	791.17	K	Joback Method
tc	1011.26	K	Joback Method
tf	463.64	K	Joback Method
vc	0.925	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	709.55	J/molxK	791.17	Joback Method
cpg	725.70	J/molxK	827.85	Joback Method
cpg	740.60	J/molxK	864.53	Joback Method
cpg	754.30	J/molxK	901.22	Joback Method
cpg	766.83	J/molxK	937.90	Joback Method
cpg	778.23	J/molxK	974.58	Joback Method
cpg	788.54	J/molxK	1011.26	Joback Method
dvisc	0.0006741	Paxs	463.64	Joback Method

dvisc	0.0003730	Paxs	518.23	Joback Method
dvisc	0.0002310	Paxs	572.82	Joback Method
dvisc	0.0001555	Paxs	627.40	Joback Method
dvisc	0.0001115	Paxs	681.99	Joback Method
dvisc	0.0000840	Paxs	736.58	Joback Method
dvisc	0.0000658	Paxs	791.17	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292654&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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