

2-Methoxybenzoic acid, 1,4-dimethylpentyl ester

Inchi:	InChI=1S/C15H22O3/c1-11(2)9-10-12(3)18-15(16)13-7-5-6-8-14(13)17-4/h5-8,11-12H,9-
InchiKey:	NDEZRZVZHZXUKH-UHFFFAOYSA-N
Formula:	C15H22O3
SMILES:	COc1ccccc1C(=O)OC(C)CCC(C)C
Mol. weight [g/mol]:	250.33

Physical Properties

Property code	Value	Unit	Source
gf	-165.60	kJ/mol	Joback Method
hf	-515.45	kJ/mol	Joback Method
hfus	25.19	kJ/mol	Joback Method
hvap	62.71	kJ/mol	Joback Method
log10ws	-4.22		Crippen Method
logp	3.677		Crippen Method
mcvol	211.760	ml/mol	McGowan Method
pc	1895.30	kPa	Joback Method
rinpol	1764.00		NIST Webbook
tb	672.09	K	Joback Method
tc	875.92	K	Joback Method
tf	362.14	K	Joback Method
vc	0.797	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.95	J/mol×K	672.09	Joback Method
cpg	649.82	J/mol×K	841.94	Joback Method
cpg	636.74	J/mol×K	807.97	Joback Method
cpg	622.73	J/mol×K	774.00	Joback Method
cpg	607.76	J/mol×K	740.03	Joback Method
cpg	591.84	J/mol×K	706.06	Joback Method
cpg	661.98	J/mol×K	875.92	Joback Method
dvisc	0.0000909	Pa×s	672.09	Joback Method
dvisc	0.0001204	Pa×s	620.43	Joback Method

dvisc	0.0001679	Pa×s	568.77	Joback Method
dvisc	0.0002501	Pa×s	517.12	Joback Method
dvisc	0.0004072	Pa×s	465.46	Joback Method
dvisc	0.0007488	Pa×s	413.80	Joback Method
dvisc	0.0016383	Pa×s	362.14	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374942&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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