

m-Methoxybenzoic acid, hexyl ester

Inchi:	InChI=1S/C14H20O3/c1-3-4-5-6-10-17-14(15)12-8-7-9-13(11-12)16-2/h7-9,11H,3-6,10H
InchiKey:	ROTBPRMBAFUZES-UHFFFAOYSA-N
Formula:	C14H20O3
SMILES:	CCCCCCOC(=O)c1cccc(OC)c1
Mol. weight [g/mol]:	236.31

Physical Properties

Property code	Value	Unit	Source
gf	-169.14	kJ/mol	Joback Method
hf	-484.25	kJ/mol	Joback Method
hfus	29.64	kJ/mol	Joback Method
hvap	61.26	kJ/mol	Joback Method
log10ws	-3.93		Crippen Method
logp	3.432		Crippen Method
mcvol	197.670	ml/mol	McGowan Method
pc	2034.55	kPa	Joback Method
rinpol	1811.80		NIST Webbook
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tb	650.09	K	Joback Method
tc	849.38	K	Joback Method
tf	380.87	K	Joback Method
vc	0.753	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.01	J/molxK	650.09	Joback Method
cpg	591.63	J/molxK	816.17	Joback Method
cpg	579.17	J/molxK	782.95	Joback Method
cpg	565.89	J/molxK	749.74	Joback Method
cpg	551.77	J/molxK	716.52	Joback Method
cpg	536.82	J/molxK	683.31	Joback Method
cpg	603.27	J/molxK	849.38	Joback Method
dvisc	0.0001181	Paxs	650.09	Joback Method

dvisc	0.0001501	Paxs	605.22	Joback Method
dvisc	0.0001982	Paxs	560.35	Joback Method
dvisc	0.0002748	Paxs	515.48	Joback Method
dvisc	0.0004053	Paxs	470.61	Joback Method
dvisc	0.0006488	Paxs	425.74	Joback Method
dvisc	0.0011604	Paxs	380.87	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U292367&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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