

m-Methoxybenzoic acid, octyl ester

Inchi:	InChI=1S/C16H24O3/c1-3-4-5-6-7-8-12-19-16(17)14-10-9-11-15(13-14)18-2/h9-11,13H,3
InchiKey:	LYMZTVMNABDKCQ-UHFFFAOYSA-N
Formula:	C16H24O3
SMILES:	CCCCCCCCOC(=O)c1cccc(OC)c1
Mol. weight [g/mol]:	264.36

Physical Properties

Property code	Value	Unit	Source
gf	-152.30	kJ/mol	Joback Method
hf	-525.53	kJ/mol	Joback Method
hfus	34.82	kJ/mol	Joback Method
hvap	65.71	kJ/mol	Joback Method
log10ws	-4.76		Crippen Method
logp	4.213		Crippen Method
mcvol	225.850	ml/mol	McGowan Method
pc	1723.16	kPa	Joback Method
rinpol	2031.90		NIST Webbook
tb	695.85	K	Joback Method
tc	890.88	K	Joback Method
tf	403.41	K	Joback Method
vc	0.866	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	628.30	J/mol×K	695.85	Joback Method
cpg	702.45	J/mol×K	858.37	Joback Method
cpg	689.41	J/mol×K	825.87	Joback Method
cpg	675.49	J/mol×K	793.36	Joback Method
cpg	660.67	J/mol×K	760.86	Joback Method
cpg	644.95	J/mol×K	728.35	Joback Method
cpg	714.61	J/mol×K	890.88	Joback Method
dvisc	0.0000941	Pa×s	695.85	Joback Method
dvisc	0.0001205	Pa×s	647.11	Joback Method

dvisc	0.0001608	Pa×s	598.37	Joback Method
dvisc	0.0002257	Pa×s	549.63	Joback Method
dvisc	0.0003386	Pa×s	500.89	Joback Method
dvisc	0.0005542	Pa×s	452.15	Joback Method
dvisc	0.0010218	Pa×s	403.41	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292368&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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