o-Methoxybenzoic acid, hexyl ester

Other names: hexyl o-anisate
o-Methoxybenzoic acid, hexyl ester
Inchi: InChI=1S/C14H20O3/c1-3-4-5-8-11-17-14(15)12-9-6-7-10-13(12)16-2/h6-7,9-10H,3-5,8,1
InchiKey: UMXZQFHEWNEFNM-UHFFFAOYSA-N
Formula: C14H20O3
SMILES: CCCCCCOC(=O)c1ccccc1OC
Mol. weight [g/mol]: 236.31

Physical Properties

Property code	Value	Unit	Source
af	0.7511		Cheméo Relay (1.0)
hf	-523.73	kJ/mol	Cheméo Relay (1.0)
hfus	29.64	kJ/mol	Joback Method
hvap	77.68	kJ/mol	Cheméo Relay (1.0)
log10ws	-4.32		Cheméo Relay (1.0)
logp	3.432		Crippen Method
mcvol	197.670	ml/mol	McGowan Method
pc	2034.55	kPa	Joback Method
rinpol	1788.10		NIST Webbook
rinpol	1788.10		NIST Webbook
tb	584.62	K	Cheméo Relay (1.0)
tc	772.84	K	Cheméo Relay (1.0)
tf	262.79	K	Cheméo Relay (1.0)
vc	0.739	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.01	J/mol×K	650.09	Joback Method
cpg	603.27	J/mol×K	849.38	Joback Method
cpg	591.63	J/mol×K	816.17	Joback Method
cpg	579.17	J/mol×K	782.95	Joback Method
cpg	565.89	J/mol×K	749.74	Joback Method
cpg	551.77	J/mol×K	716.52	Joback Method

cpg	536.82	J/mol×K	683.31	Joback Method
dvisc	0.0002748	Pa×s	515.48	Joback Method
dvisc	0.0001181	Pa×s	650.09	Joback Method
dvisc	0.0001501	Pa×s	605.22	Joback Method
dvisc	0.0001982	Pa×s	560.35	Joback Method
dvisc	0.0011604	Pa×s	380.87	Joback Method
dvisc	0.0004053	Pa×s	470.61	Joback Method
dvisc	0.0006488	Pa×s	425.74	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C71605884&Units=SI

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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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