Benzoic acid, 2-methoxy-, hexyl ester

Other names: o-Methoxybenzoic acid, hexyl ester
hexyl o-anisate
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
CAS: 71605-88-4

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	1788.10		NIST Webbook
rinpol	1788.10		NIST Webbook
tb	650.09	K	Joback Method
tc	849.38	K	Joback Method
tf	380.87	K	Joback Method
vc	0.753	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.01	J/mol×K	650.09	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
cpg	603.27	J/mol×K	849.38	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	0.0002748	Pa×s	515.48	Joback Method
dvisc	0.0004053	Pa×s	470.61	Joback Method
dvisc	0.0006488	Pa×s	425.74	Joback Method
dvisc	0.0011604	Pa×s	380.87	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C71605884&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
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