Hexyl methyl phthalate

Other names: 1,2-Benzenedicarboxylic acid, hexyl methyl ester
Inchi: InChI=1S/C15H20O4/c1-3-4-5-8-11-19-15(17)13-10-7-6-9-12(13)14(16)18-2/h6-7,9-10H,
InchiKey: XXLNRTDEQNSKEZ-UHFFFAOYSA-N
Formula: C15H20O4
SMILES: CCCCCCOC(=O)c1ccccc1C(=O)OC
Mol. weight [g/mol]: 264.32

Physical Properties

Property code	Value	Unit	Source
gf	-289.64	kJ/mol	Joback Method
hf	-617.47	kJ/mol	Joback Method
hfus	33.83	kJ/mol	Joback Method
hvap	70.23	kJ/mol	Joback Method
log10ws	-4.05		Crippen Method
logp	3.210		Crippen Method
mcvol	213.330	ml/mol	McGowan Method
pc	1975.31	kPa	Joback Method
rinpol	1938.00		NIST Webbook
rinpol	1848.00		NIST Webbook
rinpol	1848.00		NIST Webbook
tb	726.84	K	Joback Method
tc	930.46	K	Joback Method
tf	442.07	K	Joback Method
vc	0.816	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	593.63	J/mol×K	726.84	Joback Method
cpg	608.41	J/mol×K	760.78	Joback Method
cpg	622.26	J/mol×K	794.71	Joback Method
cpg	635.18	J/mol×K	828.65	Joback Method
cpg	647.19	J/mol×K	862.59	Joback Method
cpg	658.30	J/mol×K	896.52	Joback Method

cpg	668.51	J/mol×K	930.46	Joback Method
dvisc	0.0009203	Pa×s	442.07	Joback Method
dvisc	0.0005387	Pa×s	489.53	Joback Method
dvisc	0.0003467	Pa×s	536.99	Joback Method
dvisc	0.0002396	Pa×s	584.46	Joback Method
dvisc	0.0001751	Pa×s	631.92	Joback Method
dvisc	0.0001337	Pa×s	679.38	Joback Method
dvisc	0.0001057	Pa×s	726.84	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373897&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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