Benzoic acid, 3-methylphenyl ester

Inchi: InChI=1S/C14H12O2/c1-11-6-5-9-13(10-11)16-14(15)12-7-3-2-4-8-12/h2-10H,1H3
InchiKey: XYKFCIJKMCQULO-UHFFFAOYSA-N
Formula: C14H12O2
SMILES: Cc1cccc(OC(=O)c2ccccc2)c1
Mol. weight [g/mol]: 212.24

Physical Properties

Property code	Value	Unit	Source
gf	48.27	kJ/mol	Joback Method
hf	-115.50	kJ/mol	Joback Method
hfus	22.50	kJ/mol	Joback Method
hvap	61.13	kJ/mol	Joback Method
log10ws	-4.03		Crippen Method
logp	3.214		Crippen Method
mcvol	168.040	ml/mol	McGowan Method
pc	2862.74	kPa	Joback Method
rinpol	1811.00		NIST Webbook
rinpol	1811.00		NIST Webbook
tb	654.35	K	Joback Method
tc	898.02	K	Joback Method
tf	385.06	K	Joback Method
vc	0.627	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	415.01	J/mol×K	654.35	Joback Method
cpg	430.11	J/mol×K	694.96	Joback Method
cpg	444.02	J/mol×K	735.57	Joback Method
cpg	456.81	J/mol×K	776.19	Joback Method
cpg	468.50	J/mol×K	816.80	Joback Method
cpg	479.16	J/mol×K	857.41	Joback Method
cpg	488.82	J/mol×K	898.02	Joback Method
dvisc	0.0012880	Pa×s	385.06	Joback Method

dvisc	0.0007464	Pa×s	429.94	Joback Method
dvisc	0.0004795	Pa×s	474.82	Joback Method
dvisc	0.0003325	Pa×s	519.71	Joback Method
dvisc	0.0002444	Pa×s	564.59	Joback Method
dvisc	0.0001880	Pa×s	609.47	Joback Method
dvisc	0.0001499	Pa×s	654.35	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=U357800&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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