Benzoic acid, 3-methylbutyl ester

Other names:	1-(3-Methyl)butyl benzoate
	1-Butanol, 3-methyl-, 1-benzoate
	3-Methyl-1-butyl benzoate
	3-Methylbutyl benzoate
	Benzoic acid isoamyl ester
	Benzoic acid, 1-(3-methyl)butyl ester
	Benzoic acid, isopentyl ester
	Isoamyl benzoate
	Isopentyl alcohol, benzoate
	Isopentyl benzoate
	NSC 9284
Inchi:	InChI=1S/C12H16O2/c1-10(2)8-9-14-12(13)11-6-4-3-5-7-11/h3-7,10H,8-9H2,1-2H3
InchiKey:	MLLAPOCBLWUFAP-UHFFFAOYSA-N
Formula:	C12H16O2
SMILES:	CC(C)CCOC(=O)c1ccccc1
Mol. weight [g/mol]:	192.25
CAS:	54846-63-8

Physical Properties

Property code	Value	Unit	Source
af	0.5761		Cheméo Relay (1.0)
hf	-354.96	kJ/mol	Cheméo Relay (1.0)
hfus	20.14	kJ/mol	Joback Method
hvap	67.35	kJ/mol	Cheméo Relay (1.0)
ie	9.18	eV	Cheméo Relay (1.0)
log10ws	-3.75		Cheméo Relay (1.0)
logp	2.889		Crippen Method
mcvol	163.620	ml/mol	McGowan Method
pc	2537.93	kPa	Joback Method
tb	530.78	K	Cheméo Relay (1.0)
tc	725.95	K	Cheméo Relay (1.0)
tf	239.46	K	Cheméo Relay (1.0)
vc	0.596	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.41	J/mol×K	576.49	Joback Method
cpg	409.96	J/mol×K	611.54	Joback Method
cpg	424.63	J/mol×K	646.59	Joback Method
cpg	438.42	J/mol×K	681.64	Joback Method
cpg	451.37	J/mol×K	716.69	Joback Method
cpg	463.49	J/mol×K	751.74	Joback Method
cpg	474.82	J/mol×K	786.80	Joback Method
dvisc	0.0029260	Pa×s	308.58	Joback Method
dvisc	0.0013546	Pa×s	353.23	Joback Method
dvisc	0.0007455	Pa×s	397.88	Joback Method
dvisc	0.0004628	Pa×s	442.54	Joback Method
dvisc	0.0003136	Pa×s	487.19	Joback Method
dvisc	0.0002268	Pa×s	531.84	Joback Method
dvisc	0.0001725	Pa×s	576.49	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.83771e+01
Coeff. B	-8.08880e+03
Coeff. C	5.27020e+01
Temperature range (K), min.	394.45
Temperature range (K), max.	566.39

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C54846638&Units=SI

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):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume