Benzoic acid, 3-methylbut-2-yl ester

Other names: 1,2-dimethylpropyl benzoate
Benzoic acid, 3-methylbut-2-yl ester
Inchi: InChI=1S/C12H16O2/c1-9(2)10(3)14-12(13)11-7-5-4-6-8-11/h4-10H,1-3H3
InchiKey: LTUYGFZKXSBLDW-UHFFFAOYSA-N
Formula: C12H16O2
SMILES: CC(C)C(C)OC(=O)c1ccccc1
Mol. weight [g/mol]: 192.26

Physical Properties

Property code	Value	Unit	Source
af	0.5294		Cheméo Relay (1.0)
gf	-76.23	kJ/mol	Joback Method
hf	-370.49	kJ/mol	Cheméo Relay (1.0)
hfus	16.62	kJ/mol	Joback Method
hvap	66.76	kJ/mol	Cheméo Relay (1.0)
ie	9.24	eV	Cheméo Relay (1.0)
log10ws	-3.38		Cheméo Relay (1.0)
logp	2.888		Crippen Method
mcvol	163.620	ml/mol	McGowan Method
pc	2558.51	kPa	Joback Method
rinpol	1365.00		NIST Webbook
rinpol	1399.00		NIST Webbook
rinpol	1355.00		NIST Webbook
rinpol	1368.00		NIST Webbook
rinpol	1361.00		NIST Webbook
rinpol	1367.00		NIST Webbook
rinpol	1376.00		NIST Webbook
rinpol	1399.00		NIST Webbook
rinpol	1356.00		NIST Webbook
rinpol	1353.00		NIST Webbook
rinpol	1360.00		NIST Webbook
rinpol	1361.00		NIST Webbook
rinpol	1356.00		NIST Webbook
rinpol	1375.00		NIST Webbook
ripol	1840.00		NIST Webbook
ripol	1816.00		NIST Webbook
ripol	1801.00		NIST Webbook

ripol	1851.00		NIST Webbook
ripol	1827.00		NIST Webbook
ripol	1824.00		NIST Webbook
ripol	1801.00		NIST Webbook
ripol	1833.00		NIST Webbook
ripol	1825.00		NIST Webbook
ripol	1810.00		NIST Webbook
tb	518.17	K	Cheméo Relay (1.0)
tc	716.56	K	Cheméo Relay (1.0)
tf	268.28	K	Cheméo Relay (1.0)
vc	0.591	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.78	J/mol×K	576.05	Joback Method
cpg	410.72	J/mol×K	611.85	Joback Method
cpg	425.72	J/mol×K	647.64	Joback Method
cpg	439.81	J/mol×K	683.44	Joback Method
cpg	453.01	J/mol×K	719.23	Joback Method
cpg	465.34	J/mol×K	755.03	Joback Method
cpg	476.83	J/mol×K	790.82	Joback Method
dvisc	0.0039738	Pa×s	293.58	Joback Method
dvisc	0.0016112	Pa×s	340.66	Joback Method
dvisc	0.0008134	Pa×s	387.74	Joback Method
dvisc	0.0004761	Pa×s	434.81	Joback Method
dvisc	0.0003095	Pa×s	481.89	Joback Method
dvisc	0.0002172	Pa×s	528.97	Joback Method
dvisc	0.0001615	Pa×s	576.05	Joback Method

Sources

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=U367954&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

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume