

Benzoic acid, 3-methyl-, 4-methoxy-2-methylbutyl ester

Inchi:	InChI=1S/C14H20O3/c1-11-5-4-6-13(9-11)14(15)17-10-12(2)7-8-16-3/h4-6,9,12H,7-8,10
InchiKey:	FCYYUJLTAUETSX-UHFFFAOYSA-N
Formula:	C14H20O3
SMILES:	COCCC(C)COC(=O)c1cccc(C)c1
Mol. weight [g/mol]:	236.31

Physical Properties

Property code	Value	Unit	Source
gf	-171.58	kJ/mol	Joback Method
hf	-489.53	kJ/mol	Joback Method
hfus	26.12	kJ/mol	Joback Method
hvap	60.87	kJ/mol	Joback Method
log10ws	-3.13		Crippen Method
logp	2.824		Crippen Method
mvol	197.670	ml/mol	McGowan Method
pc	2049.31	kPa	Joback Method
rinpol	1797.00		NIST Webbook
rinpol	1797.00		NIST Webbook
tb	649.65	K	Joback Method
tc	852.56	K	Joback Method
tf	365.87	K	Joback Method
vc	0.748	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.47	J/molxK	649.65	Joback Method
cpg	537.60	J/molxK	683.47	Joback Method
cpg	552.84	J/molxK	717.29	Joback Method
cpg	567.20	J/molxK	751.10	Joback Method
cpg	580.68	J/molxK	784.92	Joback Method
cpg	593.31	J/molxK	818.74	Joback Method
cpg	605.07	J/molxK	852.56	Joback Method
dvisc	0.0014110	Paxs	365.87	Joback Method

dvisc	0.0007226	Paxs	413.17	Joback Method
dvisc	0.0004246	Paxs	460.46	Joback Method
dvisc	0.0002754	Paxs	507.76	Joback Method
dvisc	0.0001924	Paxs	555.06	Joback Method
dvisc	0.0001421	Paxs	602.35	Joback Method
dvisc	0.0001098	Paxs	649.65	Joback Method

Sources

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=U355710&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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