4-Methoxybenzoic acid, 3-methylbutyl ester

Other names:	4-Methoxybenzoic acid, 3-methylbutyl ester
	Benzoic acid, 4-methoxy-, 3-methylbutyl ester
	Isopentyl 4-methoxybenzoate
	isopentyl p-anisate
	Isoamyl anisate
Inchi:	InChI=1S/C13H18O3/c1-10(2)8-9-16-13(14)11-4-6-12(15-3)7-5-11/h4-7,10H,8-9H2,1-3H
InchiKey:	FVMBSMBXEVMMGH-UHFFFAOYSA-N
Formula:	C13H18O3
SMILES:	COc1ccc(C(=O)OCCC(C)C)cc1
Mol. weight [g/mol]:	222.28

Physical Properties

Property code	Value	Unit	Source
af	0.6834		Cheméo Relay (1.0)
hf	-507.83	kJ/mol	Cheméo Relay (1.0)
hfus	23.53	kJ/mol	Joback Method
hvap	76.36	kJ/mol	Cheméo Relay (1.0)
ie	8.47	eV	Cheméo Relay (1.0)
log10ws	-4.03		Cheméo Relay (1.0)
logp	2.898		Crippen Method
mcvol	183.580	ml/mol	McGowan Method
pc	2239.76	kPa	Joback Method
rinpol	1742.00		NIST Webbook
rinpol	1686.00		NIST Webbook
rinpol	1686.00		NIST Webbook
rinpol	1742.00		NIST Webbook
ripol	2333.00		NIST Webbook
tb	574.30	K	Cheméo Relay (1.0)
tc	753.28	K	Cheméo Relay (1.0)
tf	296.77	K	Cheméo Relay (1.0)
vc	0.672	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	469.86	J/mol×K	626.77	Joback Method
cpg	550.88	J/mol×K	832.59	Joback Method
cpg	539.46	J/mol×K	798.29	Joback Method
cpg	527.21	J/mol×K	763.98	Joback Method
cpg	514.14	J/mol×K	729.68	Joback Method
cpg	500.22	J/mol×K	695.38	Joback Method
cpg	485.46	J/mol×K	661.07	Joback Method
dvisc	0.0003021	Pa×s	490.69	Joback Method
dvisc	0.0001222	Pa×s	626.77	Joback Method
dvisc	0.0001577	Pa×s	581.41	Joback Method
dvisc	0.0002123	Pa×s	536.05	Joback Method
dvisc	0.0014954	Pa×s	354.60	Joback Method
dvisc	0.0004619	Pa×s	445.32	Joback Method
dvisc	0.0007775	Pa×s	399.96	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C27739293&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

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
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