Benzoic acid, 4-methoxy-, 2-methylpropyl ester

Other names: 4-Methoxybenzoic acid, 2-methylpropyl ester
iso-Butyl anisate
Isobutyl 4-methoxybenzoate
isobutyl p-anisate

Inchi: InChI=1S/C12H16O3/c1-9(2)8-15-12(13)10-4-6-11(14-3)7-5-10/h4-7,9H,8H2,1-3H3

InchiKey: HQYSDZUOGBUYJA-UHFFFAOYSA-N

Formula: C12H16O3

SMILES: COc1ccc(C(=O)OCC(C)C)cc1

Mol. weight [g/mol]: 208.25

CAS: 27739-28-2

Physical Properties

Property code	Value	Unit	Source
gf	-188.42	kJ/mol	Joback Method
hf	-448.25	kJ/mol	Joback Method
hfus	20.94	kJ/mol	Joback Method
hvap	56.42	kJ/mol	Joback Method
log10ws	-2.85		Crippen Method
logp	2.508		Crippen Method
mcvol	169.490	ml/mol	McGowan Method
pc	2458.04	kPa	Joback Method
rinpol	1629.00		NIST Webbook
rinpol	1586.00		NIST Webbook
ripol	2233.00		NIST Webbook
tb	603.89	K	Joback Method
tc	812.91	K	Joback Method
tf	343.33	K	Joback Method
vc	0.635	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	419.73	J/mol×K	603.89	Joback Method
cpg	486.66	J/mol×K	778.07	Joback Method

cpg	474.87	J/mol×K	743.24	Joback Method
cpg	462.28	J/mol×K	708.40	Joback Method
cpg	448.90	J/mol×K	673.56	Joback Method
cpg	434.72	J/mol×K	638.73	Joback Method
cpg	497.67	J/mol×K	812.91	Joback Method
dvisc	0.0001353	Pa×s	603.89	Joback Method
dvisc	0.0001738	Pa×s	560.46	Joback Method
dvisc	0.0002328	Pa×s	517.04	Joback Method
dvisc	0.0003290	Pa×s	473.61	Joback Method
dvisc	0.0004986	Pa×s	430.18	Joback Method
dvisc	0.0008297	Pa×s	386.76	Joback Method
dvisc	0.0015703	Pa×s	343.33	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C27739282&Units=SI
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

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume