Benzenebutanoic acid, 4-methoxy-, methyl ester

Other names: Butyric acid, 4-(p-methoxyphenyl)-, methyl ester
Methyl 4-(4-methoxyphenyl)butanoate
4-(4-Methoxyphenyl)butanoic acid methyl ester

Inchi: InChI=1S/C12H16O3/c1-14-11-8-6-10(7-9-11)4-3-5-12(13)15-2/h6-9H,3-5H2,1-2H3

InchiKey: FEZIYDSIDIJXQH-UHFFFAOYSA-N

Formula: C12H16O3

SMILES: COC(=O)CCCc1ccc(OC)cc1

Mol. weight [g/mol]: 208.25

CAS: 20637-08-5

Physical Properties

Property code	Value	Unit	Source
gf	-185.98	kJ/mol	Joback Method
hf	-442.97	kJ/mol	Joback Method
hfus	24.46	kJ/mol	Joback Method
hvap	56.81	kJ/mol	Joback Method
ie	7.80 ± 0.50	eV	NIST Webbook
log10ws	-2.51		Crippen Method
logp	2.191		Crippen Method
mcvol	169.490	ml/mol	McGowan Method
pc	2438.65	kPa	Joback Method
tb	604.33	K	Joback Method
tc	809.23	K	Joback Method
tf	358.33	K	Joback Method
vc	0.641	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	419.31	J/mol×K	604.33	Joback Method
cpg	484.93	J/mol×K	775.08	Joback Method
cpg	473.32	J/mol×K	740.93	Joback Method
cpg	460.95	J/mol×K	706.78	Joback Method
cpg	447.83	J/mol×K	672.63	Joback Method

cpg	433.95	J/mol×K	638.48	Joback Method
cpg	495.80	J/mol×K	809.23	Joback Method
dvisc	0.0001450	Pa×s	604.33	Joback Method
dvisc	0.0001825	Pa×s	563.33	Joback Method
dvisc	0.0002383	Pa×s	522.33	Joback Method
dvisc	0.0003255	Pa×s	481.33	Joback Method
dvisc	0.0004713	Pa×s	440.33	Joback Method
dvisc	0.0007362	Pa×s	399.33	Joback Method
dvisc	0.0012736	Pa×s	358.33	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C20637085&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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