4-(P-METHOXYPHENYL)BUTYRIC ACID

Other names: (4-Methoxyphenyl)-4-butyric acid
Benzenebutanoic acid, 4-methoxy-
Inchi: InChI=1S/C11H14O3/c1-14-10-7-5-9(6-8-10)3-2-4-11(12)13/h5-8H,2-4H2,1H3,(H,12,13)
InchiKey: LZHMNCJMXQKSBY-UHFFFAOYSA-N
Formula: C11H14O3
SMILES: COc1ccc(CCCC(=O)O)cc1
Mol. weight [g/mol]: 194.23

Physical Properties

Property code	Value	Unit	Source
hf	-495.55	kJ/mol	Cheméo Relay (1.0)
hfus	24.77	kJ/mol	Joback Method
hvap	104.53	kJ/mol	Cheméo Relay (1.0)
ie	8.17	eV	Cheméo Relay (1.0)
log10ws	-2.37		Cheméo Relay (1.0)
logp	2.102		Crippen Method
mcvol	155.400	ml/mol	McGowan Method
pc	3018.96	kPa	Joback Method
tb	600.90	K	Cheméo Relay (1.0)
tf	341.63	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.99	J/mol×K	651.21	Joback Method
cpg	410.65	J/mol×K	684.04	Joback Method
cpg	421.65	J/mol×K	716.86	Joback Method
cpg	432.01	J/mol×K	749.69	Joback Method
cpg	441.74	J/mol×K	782.51	Joback Method
cpg	450.87	J/mol×K	815.34	Joback Method
cpg	459.39	J/mol×K	848.16	Joback Method
dvisc	0.0020963	Pa×s	385.65	Joback Method
dvisc	0.0008421	Pa×s	429.91	Joback Method
dvisc	0.0004011	Pa×s	474.17	Joback Method

dvisc	0.0002168	Pa×s	518.43	Joback Method
dvisc	0.0001291	Pa×s	562.69	Joback Method
dvisc	0.0000829	Pa×s	606.95	Joback Method
dvisc	0.0000566	Pa×s	651.21	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4521282&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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point