4-(4-Methoxyphenyl)butyric acid

Other names: Benzenebutanoic acid, 4-methoxy-
(4-Methoxyphenyl)-4-butyric acid
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
CAS: 4521-28-2

Physical Properties

Property code	Value	Unit	Source
gf	-226.22	kJ/mol	Joback Method
hf	-442.34	kJ/mol	Joback Method
hfus	24.77	kJ/mol	Joback Method
hvap	68.85	kJ/mol	Joback Method
log10ws	-2.33		Crippen Method
logp	2.103		Crippen Method
mcvol	155.400	ml/mol	McGowan Method
pc	3018.96	kPa	Joback Method
tb	651.21	K	Joback Method
tc	848.16	K	Joback Method
tf	331.00 ± 0.50	K	NIST Webbook
vc	0.587	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	459.39	J/mol×K	848.16	Joback Method
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

dvisc	0.0000566	Pa×s	651.21	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
hfust	25.30	kJ/mol	330.90	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4521282&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
hfust: Enthalpy of fusion at a given temperature
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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.