

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	398.99	J/molxK	651.21	Joback Method
cpg	410.65	J/molxK	684.04	Joback Method
cpg	421.65	J/molxK	716.86	Joback Method
cpg	432.01	J/molxK	749.69	Joback Method
cpg	441.74	J/molxK	782.51	Joback Method
cpg	450.87	J/molxK	815.34	Joback Method
cpg	459.39	J/molxK	848.16	Joback Method

dvisc	0.0020963	Paxs	385.65	Joback Method
dvisc	0.0008421	Paxs	429.91	Joback Method
dvisc	0.0004011	Paxs	474.17	Joback Method
dvisc	0.0002168	Paxs	518.43	Joback Method
dvisc	0.0001291	Paxs	562.69	Joback Method
dvisc	0.0000829	Paxs	606.95	Joback Method
dvisc	0.0000566	Paxs	651.21	Joback Method
hfust	25.30	kJ/mol	330.90	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4521282&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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

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