4-(n-Butoxyphenyl)acetic acid

Other names:	4-Butoxyphenylacetic acid
	p-(Butoxyphenyl)acetic acid
	Benzeneacetic acid, 4-butoxy-
	Acetic acid, (p-butoxyphenyl)-
Inchi:	InChI=1S/C12H16O3/c1-2-3-8-15-11-6-4-10(5-7-11)9-12(13)14/h4-7H,2-3,8-9H2,1H3,(H
InchiKey:	KLJMYYFCWBVKEE-UHFFFAOYSA-N
Formula:	C12H16O3
SMILES:	CCCCOc1ccc(CC(=O)O)cc1
Mol. weight [g/mol]:	208.25
CAS:	4547-57-3

Physical Properties

Property code	Value	Unit	Source
gf	-217.80	kJ/mol	Joback Method
hf	-462.98	kJ/mol	Joback Method
hfus	27.36	kJ/mol	Joback Method
hvap	71.08	kJ/mol	Joback Method
log10ws	-2.75		Crippen Method
logp	2.493		Crippen Method
mcvol	169.490	ml/mol	McGowan Method
pc	2724.01	kPa	Joback Method
tb	674.09	K	Joback Method
tc	868.90	K	Joback Method
tf	396.92	K	Joback Method
vc	0.642	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	449.24	J/mol×K	674.09	Joback Method
cpg	461.52	J/mol×K	706.56	Joback Method
cpg	473.10	J/mol×K	739.03	Joback Method
cpg	484.01	J/mol×K	771.49	Joback Method
cpg	494.26	J/mol×K	803.96	Joback Method

cpg	503.87	J/mol×K	836.43	Joback Method
cpg	512.85	J/mol×K	868.90	Joback Method
dvisc	0.0018159	Pa×s	396.92	Joback Method
dvisc	0.0007222	Pa×s	443.12	Joback Method
dvisc	0.0003419	Pa×s	489.31	Joback Method
dvisc	0.0001841	Pa×s	535.50	Joback Method
dvisc	0.0001094	Pa×s	581.70	Joback Method
dvisc	0.0000702	Pa×s	627.89	Joback Method
dvisc	0.0000478	Pa×s	674.09	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4547573&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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