Benzeneacetic acid, butyl ester

Other names:	Acetic acid, phenyl-, butyl ester
	Butyl phenylacetate
	Phenylethanoic acid butyl ester
	Butyl benzene acetate
	n-Butyl phenylacetate
	Phenylacetic acid butyl ester
Inchi:	InChI=1S/C12H16O2/c1-2-3-9-14-12(13)10-11-7-5-4-6-8-11/h4-8H,2-3,9-10H2,1H3
InchiKey:	LDOXTQYWWYXYSQ-UHFFFAOYSA-N
Formula:	C12H16O2
SMILES:	CCCCOC(=O)Cc1ccccc1
Mol. weight [g/mol]:	192.25
CAS:	122-43-0

Physical Properties

Property code	Value	Unit	Source
gf	-71.35	kJ/mol	Joback Method
hf	-299.28	kJ/mol	Joback Method
hfus	23.66	kJ/mol	Joback Method
hvap	53.74	kJ/mol	Joback Method
log10ws	-2.81		Crippen Method
logp	2.572		Crippen Method
mcvol	163.620	ml/mol	McGowan Method
pc	2517.59	kPa	Joback Method
rinpol	1446.00		NIST Webbook
rinpol	1407.64		NIST Webbook
rinpol	1433.00		NIST Webbook
rinpol	1420.00		NIST Webbook
rinpol	1407.64		NIST Webbook
rinpol	1408.00		NIST Webbook
rinpol	1408.00		NIST Webbook
rinpol	1446.00		NIST Webbook
ripol	1970.00		NIST Webbook
ripol	1932.00		NIST Webbook
ripol	1932.00		NIST Webbook
ripol	1970.00		NIST Webbook
tb	576.93	K	Joback Method
tc	782.93	K	Joback Method

tf	323.58	K	Joback Method
vc	0.624	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.04	J/mol×K	576.93	Joback Method
cpg	409.22	J/mol×K	611.26	Joback Method
cpg	423.55	J/mol×K	645.60	Joback Method
cpg	437.06	J/mol×K	679.93	Joback Method
cpg	449.76	J/mol×K	714.26	Joback Method
cpg	461.69	J/mol×K	748.60	Joback Method
cpg	472.86	J/mol×K	782.93	Joback Method
dvisc	0.0022442	Pa×s	323.58	Joback Method
dvisc	0.0011633	Pa×s	365.81	Joback Method
dvisc	0.0006908	Pa×s	408.03	Joback Method
dvisc	0.0004524	Pa×s	450.25	Joback Method
dvisc	0.0003185	Pa×s	492.48	Joback Method
dvisc	0.0002371	Pa×s	534.70	Joback Method
dvisc	0.0001842	Pa×s	576.93	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=C122430&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume