

4-Butylbenzoic acid, ethyl ester

Inchi:	InChI=1S/C13H18O2/c1-3-5-6-11-7-9-12(10-8-11)13(14)15-4-2/h7-10H,3-6H2,1-2H3
InchiKey:	NKAVJELRFJVPEE-UHFFFAOYSA-N
Formula:	C13H18O2
SMILES:	CCCCc1ccc(C(=O)OCC)cc1
Mol. weight [g/mol]:	206.28
CAS:	85100-62-5

Physical Properties

Property code	Value	Unit	Source
gf	-72.56	kJ/mol	Joback Method
hf	-331.39	kJ/mol	Joback Method
hfus	25.86	kJ/mol	Joback Method
hvap	56.63	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	3.206		Crippen Method
mcvol	177.710	ml/mol	McGowan Method
pc	2258.96	kPa	Joback Method
rinpol	1623.70		NIST Webbook
rinpol	1623.70		NIST Webbook
tb	604.79	K	Joback Method
tc	808.65	K	Joback Method
tf	347.37	K	Joback Method
vc	0.679	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	443.04	J/molxK	604.79	Joback Method
cpg	458.61	J/molxK	638.77	Joback Method
cpg	473.35	J/molxK	672.74	Joback Method
cpg	487.26	J/molxK	706.72	Joback Method
cpg	500.37	J/molxK	740.70	Joback Method
cpg	512.69	J/molxK	774.67	Joback Method
cpg	524.25	J/molxK	808.65	Joback Method

dvisc	0.0016609	Paxs	347.37	Joback Method
dvisc	0.0009147	Paxs	390.27	Joback Method
dvisc	0.0005669	Paxs	433.18	Joback Method
dvisc	0.0003830	Paxs	476.08	Joback Method
dvisc	0.0002761	Paxs	518.98	Joback Method
dvisc	0.0002092	Paxs	561.89	Joback Method
dvisc	0.0001649	Paxs	604.79	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C85100625&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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