ETHYL P-(BUTYLAMINO)BENZOATE

Other names: Benzoic acid, 4-(butylamino)-, ethyl ester
Ethyl p-butylaminobenzoate
Inchi: InChI=1S/C13H19NO2/c1-3-5-10-14-12-8-6-11(7-9-12)13(15)16-4-2/h6-9,14H,3-5,10H2,
InchiKey: GTXRSQYDLPYYNW-UHFFFAOYSA-N
Formula: C13H19NO2
SMILES: CCCCNc1ccc(C(=O)OCC)cc1
Mol. weight [g/mol]: 221.30

Physical Properties

Property code	Value	Unit	Source
af	0.7114		Cheméo Relay (1.0)
hf	-383.63	kJ/mol	Cheméo Relay (1.0)
hfus	30.96	kJ/mol	Joback Method
hvap	80.71	kJ/mol	Cheméo Relay (1.0)
ie	7.44	eV	Cheméo Relay (1.0)
log10ws	-4.04		Cheméo Relay (1.0)
logp	3.075		Crippen Method
mcvol	187.690	ml/mol	McGowan Method
pc	2287.14	kPa	Joback Method
rinpol	2148.00		NIST Webbook
rinpol	2170.00		NIST Webbook
rinpol	2158.00		NIST Webbook
rinpol	2148.00		NIST Webbook
tb	592.38	K	Cheméo Relay (1.0)
tc	788.15	K	Cheméo Relay (1.0)
tf	314.69	K	Cheméo Relay (1.0)
vc	0.684	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	496.54	J/mol×K	654.96	Joback Method
cpg	511.74	J/mol×K	688.96	Joback Method
cpg	526.06	J/mol×K	722.95	Joback Method

cpg	539.54	J/mol×K	756.95	Joback Method
cpg	552.17	J/mol×K	790.95	Joback Method
cpg	564.00	J/mol×K	824.95	Joback Method
cpg	575.04	J/mol×K	858.94	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C94326&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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