

BUTYL ANTHRANILATE

Other names:	Benzoic acid, 2-amino-, butyl ester
Inchi:	InChI=1S/C11H15NO2/c1-2-3-8-14-11(13)9-6-4-5-7-10(9)12/h4-7H,2-3,8,12H2,1H3
InchiKey:	HUIYGGQINIVDNW-UHFFFAOYSA-N
Formula:	C11H15NO2
SMILES:	CCCCOC(=O)c1ccccc1N
Mol. weight [g/mol]:	193.25

Physical Properties

Property code	Value	Unit	Source
af	0.6878		Cheméo Relay (1.0)
hf	-354.30	kJ/mol	Cheméo Relay (1.0)
hfus	25.88	kJ/mol	Joback Method
hvap	72.69	kJ/mol	Cheméo Relay (1.0)
ie	7.91	eV	Cheméo Relay (1.0)
log10ws	-3.59		Cheméo Relay (1.0)
logp	2.226		Crippen Method
mcvol	159.510	ml/mol	McGowan Method
pc	2906.11	kPa	Joback Method
rinpol	1600.00		NIST Webbook
ripol	2419.00		NIST Webbook
tb	574.85	K	Cheméo Relay (1.0)
tc	775.53	K	Cheméo Relay (1.0)
tf	265.91	K	Cheméo Relay (1.0)
vc	0.577	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	405.64	J/mol×K	631.56	Joback Method
cpg	419.40	J/mol×K	667.92	Joback Method
cpg	432.33	J/mol×K	704.28	Joback Method
cpg	444.44	J/mol×K	740.64	Joback Method
cpg	455.75	J/mol×K	777.00	Joback Method
cpg	466.27	J/mol×K	813.36	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=C7756969&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/ci990307I

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

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