Benzoic acid, 2-[(phenylmethyl)amino]-

Other names:	Anthranilic acid, N-benzyl-
	N-Benzylanthranilic acid
	N-Benzyl-o-aminobenzoic acid
	2-[(phenylmethyl)amino]benzoic acid
Inchi:	InChI=1S/C14H13NO2/c16-14(17)12-8-4-5-9-13(12)15-10-11-6-2-1-3-7-11/h1-9,15H,10H
InchiKey:	JGQKORRBYIBYOF-UHFFFAOYSA-N
Formula:	C14H13NO2
SMILES:	O=C(O)c1ccccc1NCc1ccccc1
Mol. weight [g/mol]:	227.26
CAS:	6622-55-5

Physical Properties

Property code	Value	Unit	Source
gf	105.84	kJ/mol	Joback Method
hf	-82.04	kJ/mol	Joback Method
hfus	30.50	kJ/mol	Joback Method
hvap	81.83	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	2.997		Crippen Method
mcvol	178.020	ml/mol	McGowan Method
pc	3276.53	kPa	Joback Method
tb	774.28	K	Joback Method
tc	999.51	K	Joback Method
tf	476.31	K	Joback Method
vc	0.663	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	490.01	J/mol×K	774.28	Joback Method
cpg	501.42	J/mol×K	811.82	Joback Method
cpg	511.92	J/mol×K	849.36	Joback Method
cpg	521.56	J/mol×K	886.90	Joback Method
cpg	530.42	J/mol×K	924.43	Joback Method

cpg	538.54	J/mol×K	961.97	Joback Method
cpg	546.00	J/mol×K	999.51	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=C6622555&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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