Benzoic acid, 2-amino-, 2-phenylethyl ester

Other names:	Anthranilic acid, phenethyl ester
	Benzylcarbinyl anthranilate
	Phenethyl anthranilate
	Phenylethyl anthranilate
	2-Phenylethyl anthranilate
	2-Phenylethyl o-aminobenzoate
	«beta»-Phenylethyl anthranilate
	«beta»-Phenethyl o-aminobenzoate
	2-Phenylethyl 2-aminobenzoate
	Anthranilic acid, phenylethyl ester
	NSC 66441
Inchi:	InChI=1S/C15H15NO2/c16-14-9-5-4-8-13(14)15(17)18-11-10-12-6-2-1-3-7-12/h1-9H,10-
InchiKey:	PXWNBAGCFUDYBE-UHFFFAOYSA-N
Formula:	C15H15NO2
SMILES:	Nc1ccccc1C(=O)OCCc1ccccc1
Mol. weight [g/mol]:	241.29
CAS:	133-18-6

Physical Properties

Property code	Value	Unit	Source
gf	123.14	kJ/mol	Joback Method
hf	-102.35	kJ/mol	Joback Method
hfus	30.28	kJ/mol	Joback Method
hvap	74.00	kJ/mol	Joback Method
log10ws	-3.38		Crippen Method
logp	2.668		Crippen Method
mcvol	192.110	ml/mol	McGowan Method
pc	2746.90	kPa	Joback Method
rinpol	2091.00		NIST Webbook
rinpol	2120.00		NIST Webbook
rinpol	2088.00		NIST Webbook
rinpol	2120.00		NIST Webbook
rinpol	2088.00		NIST Webbook
rinpol	2088.00		NIST Webbook
rinpol	2080.00		NIST Webbook
rinpol	2091.00		NIST Webbook
tb	749.76	K	Joback Method

tc	993.25	K	Joback Method
tf	479.59	K	Joback Method
vc	0.713	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	526.49	J/mol×K	749.76	Joback Method
cpg	540.79	J/mol×K	790.34	Joback Method
cpg	553.88	J/mol×K	830.92	Joback Method
cpg	565.80	J/mol×K	871.51	Joback Method
cpg	576.63	J/mol×K	912.09	Joback Method
cpg	586.42	J/mol×K	952.67	Joback Method
cpg	595.22	J/mol×K	993.25	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C133186&Units=SI

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
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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