Benzoic acid, 2-amino-, phenylmethyl ester

Other names: Benzyl anthranilate
Inchi: InChI=1S/C14H13NO2/c15-13-9-5-4-8-12(13)14(16)17-10-11-6-2-1-3-7-11/h1-9H,10,15H
InchiKey: ZHZPDMZPDWXVMJ-UHFFFAOYSA-N
Formula: C14H13NO2
SMILES: Nc1ccccc1C(=O)OCc1ccccc1
Mol. weight [g/mol]: 227.26
CAS: 82185-41-9

Physical Properties

Property code	Value	Unit	Source
gf	114.72	kJ/mol	Joback Method
hf	-81.71	kJ/mol	Joback Method
hfus	27.69	kJ/mol	Joback Method
hvap	71.77	kJ/mol	Joback Method
log10ws	-3.46		Crippen Method
logp	2.626		Crippen Method
mcvol	178.020	ml/mol	McGowan Method
pc	3045.68	kPa	Joback Method
tb	726.88	K	Joback Method
tc	975.56	K	Joback Method
tf	468.32	K	Joback Method
vc	0.656	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	473.91	J/mol×K	726.88	Joback Method
cpg	487.82	J/mol×K	768.33	Joback Method
cpg	500.54	J/mol×K	809.77	Joback Method
cpg	512.10	J/mol×K	851.22	Joback Method
cpg	522.57	J/mol×K	892.67	Joback Method
cpg	532.01	J/mol×K	934.11	Joback Method
cpg	540.46	J/mol×K	975.56	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C82185419&Units=SI
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

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