

Benzoic acid, 2-amino-, pentyl ester

Other names:	Anthranilic acid, pentyl ester Pentyl 2-aminobenzoate pentyl anthranilate
Inchi:	InChI=1S/C12H17NO2/c1-2-3-6-9-15-12(14)10-7-4-5-8-11(10)13/h4-5,7-8H,2-3,6,9,13H2
InchiKey:	JCKCYPSMCQDSHT-UHFFFAOYSA-N
Formula:	C12H17NO2
SMILES:	CCCCCOC(=O)c1cccc1N
Mol. weight [g/mol]:	207.27
CAS:	30100-15-3

Physical Properties

Property code	Value	Unit	Source
gf	-14.53	kJ/mol	Joback Method
hf	-276.96	kJ/mol	Joback Method
hfus	28.47	kJ/mol	Joback Method
hvap	65.04	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	2.616		Crippen Method
mcvol	173.600	ml/mol	McGowan Method
pc	2627.15	kPa	Joback Method
rinpol	1700.00		NIST Webbook
rinpol	1753.00		NIST Webbook
rinpol	1700.00		NIST Webbook
rinpol	1753.00		NIST Webbook
ripol	2510.00		NIST Webbook
ripol	2510.00		NIST Webbook
tb	654.44	K	Joback Method
tc	868.94	K	Joback Method
tf	419.36	K	Joback Method
vc	0.652	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	455.70	J/mol×K	654.44	Joback Method
cpg	470.08	J/mol×K	690.19	Joback Method
cpg	483.58	J/mol×K	725.94	Joback Method
cpg	496.23	J/mol×K	761.69	Joback Method
cpg	508.05	J/mol×K	797.44	Joback Method
cpg	519.05	J/mol×K	833.19	Joback Method
cpg	529.27	J/mol×K	868.94	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=C30100153&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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