

2-aminobenzaldehyde

Other names:	Benzaldehyde, 2-amino-
Inchi:	InChI=1S/C7H7NO/c8-7-4-2-1-3-6(7)5-9/h1-5H,8H2
InchiKey:	FXWFZIRWWNPPOV-UHFFFAOYSA-N
Formula:	C7H7NO
SMILES:	Nc1cccc1C=O
Mol. weight [g/mol]:	121.14
CAS:	529-23-7

Physical Properties

Property code	Value	Unit	Source
gf	77.77	kJ/mol	Joback Method
hf	-14.54	kJ/mol	Joback Method
hfus	15.02	kJ/mol	Joback Method
hvap	51.48	kJ/mol	Joback Method
log10ws	-1.35		Crippen Method
logp	1.081		Crippen Method
mcvol	97.280	ml/mol	McGowan Method
pc	4802.50	kPa	Joback Method
rinpol	1222.00		NIST Webbook
tb	512.41	K	Joback Method
tc	744.79	K	Joback Method
tf	313.00	K	NIST Webbook
vc	0.365	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	202.34	J/molxK	512.41	Joback Method
cpg	212.25	J/molxK	551.14	Joback Method
cpg	221.48	J/molxK	589.87	Joback Method
cpg	230.08	J/molxK	628.60	Joback Method
cpg	238.07	J/molxK	667.33	Joback Method
cpg	245.48	J/molxK	706.06	Joback Method
cpg	252.33	J/molxK	744.79	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	355.50 ± 2.50	K	0.30	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C529237&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
mvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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