3-Aminobenzyl alcohol

Other names: Benzyl alcohol, m-amino-
m-Aminobenzyl alcohol
3-Aminobenzyl alcohol
m-Aminophenylcarbinol
Inchi: InChI=1S/C7H9NO/c8-7-3-1-2-6(4-7)5-9/h1-4,9H,5,8H2
InchiKey: OJZQOQNSUZLSMV-UHFFFAOYSA-N
Formula: C7H9NO
SMILES: Nc1cccc(CO)c1
Mol. weight [g/mol]: 123.15

Physical Properties

Property code	Value	Unit	Source
af	0.6718		Cheméo Relay (1.0)
hf	-94.65	kJ/mol	Cheméo Relay (1.0)
hfus	16.82	kJ/mol	Joback Method
hvap	83.47	kJ/mol	Cheméo Relay (1.0)
ie	8.12	eV	Cheméo Relay (1.0)
log10ws	-0.25		Cheméo Relay (1.0)
logp	0.761		Crippen Method
mcvol	101.580	ml/mol	McGowan Method
pc	4924.59	kPa	Joback Method
tb	542.90	K	Cheméo Relay (1.0)
tc	820.33	K	Cheméo Relay (1.0)
tf	318.81	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	230.88	J/mol×K	555.93	Joback Method
cpg	240.23	J/mol×K	591.16	Joback Method
cpg	249.02	J/mol×K	626.39	Joback Method
cpg	257.26	J/mol×K	661.62	Joback Method
cpg	264.99	J/mol×K	696.85	Joback Method
cpg	272.21	J/mol×K	732.09	Joback Method

cpg	278.97	J/mol×K	767.32	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1877776&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
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