Benzen-d5-amine

Other names: Aniline-d5
[2,3,4,5,6-2H5]aniline
aniline-2,3,4,5,6-d5
Inchi: InChI=1S/C6H7N/c7-6-4-2-1-3-5-6/h1-5H,7H2/i1D,2D,3D,4D,5D
InchiKey: PAYRUJLWNCNPSJ-RALIUCGRSA-N
Formula: C6H2D5N
SMILES: Nc1ccccc1
Mol. weight [g/mol]: 98.16
CAS: 4165-61-1

Physical Properties

Property code	Value	Unit	Source
gf	178.50	kJ/mol	Joback Method
hf	103.15	kJ/mol	Joback Method
hfus	10.53	kJ/mol	Joback Method
hvap	41.87	kJ/mol	Joback Method
log10ws	-1.11		Crippen Method
logp	1.269		Crippen Method
mcvol	81.620	ml/mol	McGowan Method
pc	5058.59	kPa	Joback Method
tb	435.89	K	Joback Method
tc	666.01	K	Joback Method
tf	267.06	K	Joback Method
vc	0.292	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	149.06	J/mol×K	435.89	Joback Method
cpg	159.56	J/mol×K	474.24	Joback Method
cpg	169.35	J/mol×K	512.60	Joback Method
cpg	178.46	J/mol×K	550.95	Joback Method
cpg	186.94	J/mol×K	589.30	Joback Method
cpg	194.81	J/mol×K	627.66	Joback Method

cpg	202.11	J/mol×K	666.01	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Deuterium isotope effects in liquid liquid phase diagrams of aniline + cyclohexane mixtures:	https://www.doi.org/10.1016/j.fluid.2005.10.002
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=C4165611&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume