Benzenamine, 2-(1-methylethenyl)-

Other names: o-Isopropenylaniline
2-Isopropenylaniline
Inchi: InChI=1S/C9H11N/c1-7(2)8-5-3-4-6-9(8)10/h3-6H,1,10H2,2H3
InchiKey: HEDYZFYQYPWWCC-UHFFFAOYSA-N
Formula: C9H11N
SMILES: C=C(C)c1ccccc1N
Mol. weight [g/mol]: 133.19
CAS: 52562-19-3

Physical Properties

Property code	Value	Unit	Source
gf	273.42	kJ/mol	Joback Method
hf	145.40	kJ/mol	Joback Method
hfus	15.32	kJ/mol	Joback Method
hvap	48.62	kJ/mol	Joback Method
log10ws	-2.35		Crippen Method
logp	2.302		Crippen Method
mcvol	119.590	ml/mol	McGowan Method
pc	3620.24	kPa	Joback Method
tb	506.07	K	Joback Method
tc	736.19	K	Joback Method
tf	297.67	K	Joback Method
vc	0.443	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	253.38	J/mol×K	506.07	Joback Method
cpg	266.55	J/mol×K	544.42	Joback Method
cpg	278.87	J/mol×K	582.78	Joback Method
cpg	290.36	J/mol×K	621.13	Joback Method
cpg	301.09	J/mol×K	659.48	Joback Method
cpg	311.08	J/mol×K	697.83	Joback Method
cpg	320.39	J/mol×K	736.19	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	368.20	K	1.70	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C52562193&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume