Benzenamine, 4-propoxy-

Other names:	p-Propoxyaniline
	4-n-Propoxyaniline
	4-propoxyaniline
Inchi:	InChI=1S/C9H13NO/c1-2-7-11-9-5-3-8(10)4-6-9/h3-6H,2,7,10H2,1H3
InchiKey:	DWOIGSLSPPLRKO-UHFFFAOYSA-N
Formula:	C9H13NO
SMILES:	CCCOc1ccc(N)cc1
Mol. weight [g/mol]:	151.21
CAS:	4469-80-1

Physical Properties

Property code	Value	Unit	Source
gf	89.13	kJ/mol	Joback Method
hf	-102.46	kJ/mol	Joback Method
hfus	19.10	kJ/mol	Joback Method
hvap	51.62	kJ/mol	Joback Method
log10ws	-2.06		Crippen Method
logp	2.058		Crippen Method
mcvol	129.760	ml/mol	McGowan Method
pc	3356.75	kPa	Joback Method
tb	531.93	K	Joback Method
tc	750.09	K	Joback Method
tf	335.62	K	Joback Method
vc	0.478	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	295.02	J/mol×K	531.93	Joback Method
cpg	308.41	J/mol×K	568.29	Joback Method
cpg	321.08	J/mol×K	604.65	Joback Method
cpg	333.04	J/mol×K	641.01	Joback Method
cpg	344.32	J/mol×K	677.37	Joback Method
cpg	354.92	J/mol×K	713.73	Joback Method

cpg	364.86	J/mol×K	750.09	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	414.00 ± 1.00	K	2.00	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=C4469801&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

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