Aniline, N-(3-bromopropyl)-N-methyl-

Inchi: InChI=1S/C10H14BrN/c1-12(9-5-8-11)10-6-3-2-4-7-10/h2-4,6-7H,5,8-9H2,1H3
InchiKey: YWVIBERYLABRBJ-UHFFFAOYSA-N
Formula: C10H14BrN
SMILES: CN(CCCBr)c1ccccc1
Mol. weight [g/mol]: 228.13

Physical Properties

Property code	Value	Unit	Source
gf	270.83	kJ/mol	Joback Method
hf	80.66	kJ/mol	Joback Method
hfus	24.00	kJ/mol	Joback Method
hvap	48.61	kJ/mol	Joback Method
log10ws	-2.65		Crippen Method
logp	2.908		Crippen Method
mcvol	155.480	ml/mol	McGowan Method
pc	3156.17	kPa	Joback Method
rinpol	1649.00		NIST Webbook
tb	533.48	K	Joback Method
tc	750.96	K	Joback Method
tf	321.15	K	Joback Method
vc	0.568	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	332.42	J/mol×K	533.48	Joback Method
cpg	347.38	J/mol×K	569.73	Joback Method
cpg	361.33	J/mol×K	605.97	Joback Method
cpg	374.32	J/mol×K	642.22	Joback Method
cpg	386.42	J/mol×K	678.46	Joback Method
cpg	397.68	J/mol×K	714.71	Joback Method
cpg	408.16	J/mol×K	750.96	Joback Method

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=U380552&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume