2,6-Dibromo-4-isopropylaniline

Inchi: InChI=1S/C9H11Br2N/c1-5(2)6-3-7(10)9(12)8(11)4-6/h3-5H,12H2,1-2H3
InchiKey: CJEBZUFROMNDEK-UHFFFAOYSA-N
Formula: C9H11Br2N
SMILES: CC(C)c1cc(Br)c(N)c(Br)c1
Mol. weight [g/mol]: 293.00
CAS: 10546-65-3

Physical Properties

Property code	Value	Unit	Source
gf	201.07	kJ/mol	Joback Method
hf	54.20	kJ/mol	Joback Method
hfus	24.18	kJ/mol	Joback Method
hvap	63.01	kJ/mol	Joback Method
log10ws	-4.62		Crippen Method
logp	3.917		Crippen Method
mcvol	158.890	ml/mol	McGowan Method
pc	3940.66	kPa	Joback Method
tb	651.35	K	Joback Method
tc	906.43	K	Joback Method
tf	443.03	K	Joback Method
vc	0.579	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	339.33	J/mol×K	651.35	Joback Method
cpg	350.52	J/mol×K	693.86	Joback Method
cpg	360.89	J/mol×K	736.38	Joback Method
cpg	370.51	J/mol×K	778.89	Joback Method
cpg	379.44	J/mol×K	821.40	Joback Method
cpg	387.73	J/mol×K	863.92	Joback Method
cpg	395.44	J/mol×K	906.43	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10546653&Units=SI
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

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