Aniline, n-isopentyl-

Inchi: InChI=1S/C11H17N/c1-10(2)8-9-12-11-6-4-3-5-7-11/h3-7,10,12H,8-9H2,1-2H3
InchiKey: HXKYNBCJKDAHOJ-UHFFFAOYSA-N
Formula: C11H17N
SMILES: CC(C)CCNc1ccccc1
Mol. weight [g/mol]: 163.26
CAS: 2051-84-5

Physical Properties

Property code	Value	Unit	Source
gf	241.10	kJ/mol	Joback Method
hf	14.35	kJ/mol	Joback Method
hfus	19.86	kJ/mol	Joback Method
hvap	48.40	kJ/mol	Joback Method
log10ws	-2.91		Crippen Method
logp	3.145		Crippen Method
mcvol	152.070	ml/mol	McGowan Method
pc	2707.03	kPa	Joback Method
tb	529.15 ± 0.50	K	NIST Webbook
tc	735.29	K	Joback Method
tf	277.81	K	Joback Method
vc	0.573	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.84	J/mol×K	527.49	Joback Method
cpg	367.24	J/mol×K	562.12	Joback Method
cpg	382.70	J/mol×K	596.76	Joback Method
cpg	397.25	J/mol×K	631.39	Joback Method
cpg	410.92	J/mol×K	666.02	Joback Method
cpg	423.77	J/mol×K	700.66	Joback Method
cpg	435.81	J/mol×K	735.29	Joback Method

Sources

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=C2051845&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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