Aniline, n-(beta-methylallyl)-

Inchi: InChI=1S/C10H13N/c1-9(2)8-11-10-6-4-3-5-7-10/h3-7,11H,1,8H2,2H3
InchiKey: JCBGGIHYIHYKEX-UHFFFAOYSA-N
Formula: C10H13N
SMILES: C=C(C)CNc1ccccc1
Mol. weight [g/mol]: 147.22
CAS: 22774-81-8

Physical Properties

Property code	Value	Unit	Source
gf	314.41	kJ/mol	Joback Method
hf	155.91	kJ/mol	Joback Method
hfus	18.21	kJ/mol	Joback Method
hvap	45.98	kJ/mol	Joback Method
log10ws	-2.59		Crippen Method
logp	2.675		Crippen Method
mcvol	133.680	ml/mol	McGowan Method
pc	3131.49	kPa	Joback Method
tb	501.61	K	Joback Method
tc	716.54	K	Joback Method
tf	265.82	K	Joback Method
vc	0.504	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	286.27	J/mol×K	501.61	Joback Method
cpg	301.08	J/mol×K	537.43	Joback Method
cpg	314.96	J/mol×K	573.25	Joback Method
cpg	327.96	J/mol×K	609.07	Joback Method
cpg	340.11	J/mol×K	644.89	Joback Method
cpg	351.47	J/mol×K	680.72	Joback Method
cpg	362.08	J/mol×K	716.54	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=C22774818&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

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