Benzenemethanamine, «alpha»-ethyl

Inchi: InChI=1S/C9H13N/c1-2-9(10)8-6-4-3-5-7-8/h3-7,9H,2,10H2,1H3
InchiKey: AQFLVLHRZFLDDV-UHFFFAOYSA-N
Formula: C9H13N
SMILES: CCC(N)c1ccccc1
Mol. weight [g/mol]: 135.21
CAS: 2941-20-0

Physical Properties

Property code	Value	Unit	Source
gf	201.32	kJ/mol	Joback Method
hf	35.95	kJ/mol	Joback Method
hfus	14.78	kJ/mol	Joback Method
hvap	48.16	kJ/mol	Joback Method
log10ws	-2.59		Crippen Method
logp	2.096		Crippen Method
mcvol	123.890	ml/mol	McGowan Method
pc	3517.91	kPa	Joback Method
rinpol	1128.00		NIST Webbook
tb	504.09	K	Joback Method
tc	728.62	K	Joback Method
tf	285.87	K	Joback Method
vc	0.455	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	271.70	J/mol×K	504.09	Joback Method
cpg	286.20	J/mol×K	541.51	Joback Method
cpg	299.78	J/mol×K	578.93	Joback Method
cpg	312.48	J/mol×K	616.35	Joback Method
cpg	324.34	J/mol×K	653.78	Joback Method
cpg	335.40	J/mol×K	691.20	Joback Method
cpg	345.71	J/mol×K	728.62	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=C2941200&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