3-Amino-2-methylheptane

Inchi: InChI=1S/C8H19N/c1-4-5-6-8(9)7(2)3/h7-8H,4-6,9H2,1-3H3
InchiKey: WXTMKAIMGVITMT-UHFFFAOYSA-N
Formula: C8H19N
SMILES: CCCCC(N)C(C)C
Mol. weight [g/mol]: 129.24
CAS: 116557-25-6

Physical Properties

Property code	Value	Unit	Source
gf	78.05	kJ/mol	Joback Method
hf	-185.22	kJ/mol	Joback Method
hfus	14.63	kJ/mol	Joback Method
hvap	43.27	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	2.160		Crippen Method
mcvol	133.560	ml/mol	McGowan Method
pc	2732.56	kPa	Joback Method
tb	454.09	K	Joback Method
tc	639.32	K	Joback Method
tf	233.18	K	Joback Method
vc	0.500	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	292.77	J/mol×K	454.09	Joback Method
cpg	307.18	J/mol×K	484.96	Joback Method
cpg	320.97	J/mol×K	515.83	Joback Method
cpg	334.15	J/mol×K	546.71	Joback Method
cpg	346.76	J/mol×K	577.58	Joback Method
cpg	358.79	J/mol×K	608.45	Joback Method
cpg	370.27	J/mol×K	639.32	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=C116557256&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume