ethylheptyl-amine

Other names: heptanamine, N-ethyl-
Inchi: InChI=1S/C9H21N/c1-3-5-6-7-8-9-10-4-2/h10H,3-9H2,1-2H3
InchiKey: IUZZLNVABCISOI-UHFFFAOYSA-N
Formula: C9H21N
SMILES: CCCCCCCNCC
Mol. weight [g/mol]: 143.27
CAS: 66793-76-8

Physical Properties

Property code	Value	Unit	Source
gf	114.29	kJ/mol	Joback Method
hf	-175.62	kJ/mol	Joback Method
hfus	24.16	kJ/mol	Joback Method
hvap	42.06	kJ/mol	Joback Method
log10ws	-2.78		Crippen Method
logp	2.566		Crippen Method
mcvol	147.650	ml/mol	McGowan Method
pc	2336.03	kPa	Joback Method
rinpol	1056.00		NIST Webbook
tb	455.49	K	Joback Method
tc	622.89	K	Joback Method
tf	243.85	K	Joback Method
vc	0.575	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.73	J/mol×K	455.49	Joback Method
cpg	337.31	J/mol×K	483.39	Joback Method
cpg	351.32	J/mol×K	511.29	Joback Method
cpg	364.79	J/mol×K	539.19	Joback Method
cpg	377.73	J/mol×K	567.09	Joback Method
cpg	390.14	J/mol×K	594.99	Joback Method
cpg	402.06	J/mol×K	622.89	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=C66793768&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume