Ethanol, 2-(hexylamino)-

Other names: 2-hexylaminoethanol
Inchi: InChI=1S/C8H19NO/c1-2-3-4-5-6-9-7-8-10/h9-10H,2-8H2,1H3
InchiKey: MCIKGVLBLIZYRY-UHFFFAOYSA-N
Formula: C8H19NO
SMILES: CCCCCCNCCO
Mol. weight [g/mol]: 145.24
CAS: 54596-69-9

Physical Properties

Property code	Value	Unit	Source
gf	-30.95	kJ/mol	Joback Method
hf	-307.21	kJ/mol	Joback Method
hfus	25.66	kJ/mol	Joback Method
hvap	56.52	kJ/mol	Joback Method
log10ws	-1.62		Crippen Method
logp	1.149		Crippen Method
mcvol	139.430	ml/mol	McGowan Method
pc	2826.33	kPa	Joback Method
rinpol	1197.00		NIST Webbook
rinpol	1197.00		NIST Webbook
tb	524.79	K	Joback Method
tc	688.02	K	Joback Method
tf	293.40	K	Joback Method
vc	0.537	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	338.39	J/mol×K	524.79	Joback Method
cpg	350.27	J/mol×K	552.00	Joback Method
cpg	361.68	J/mol×K	579.20	Joback Method
cpg	372.63	J/mol×K	606.41	Joback Method
cpg	383.14	J/mol×K	633.61	Joback Method
cpg	393.21	J/mol×K	660.82	Joback Method

cpg	402.87	J/mol×K	688.02	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	394.50 ± 0.50	K	1.90	NIST Webbook

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=C54596699&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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume