propyloctyl-amine

Inchi: InChI=1S/C11H25N/c1-3-5-6-7-8-9-11-12-10-4-2/h12H,3-11H2,1-2H3
InchiKey: BBFLXVFMAOURDU-UHFFFAOYSA-N
Formula: C11H25N
SMILES: CCCCCCCCNCCC
Mol. weight [g/mol]: 171.32
CAS: 75898-40-7

Physical Properties

Property code	Value	Unit	Source
gf	131.13	kJ/mol	Joback Method
hf	-216.90	kJ/mol	Joback Method
hfus	29.34	kJ/mol	Joback Method
hvap	46.52	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	3.346		Crippen Method
mcvol	175.830	ml/mol	McGowan Method
pc	1956.14	kPa	Joback Method
rinpol	1246.00		NIST Webbook
tb	501.25	K	Joback Method
tc	666.61	K	Joback Method
tf	266.39	K	Joback Method
vc	0.686	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	415.42	J/mol×K	501.25	Joback Method
cpg	431.59	J/mol×K	528.81	Joback Method
cpg	447.13	J/mol×K	556.37	Joback Method
cpg	462.05	J/mol×K	583.93	Joback Method
cpg	476.37	J/mol×K	611.49	Joback Method
cpg	490.11	J/mol×K	639.05	Joback Method
cpg	503.28	J/mol×K	666.61	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=C75898407&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

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