

propylheptyl-amine

Inchi:	InChI=1S/C10H23N/c1-3-5-6-7-8-10-11-9-4-2/h11H,3-10H2,1-2H3
InchiKey:	SENZORBCFNNGDX-UHFFFAOYSA-N
Formula:	C10H23N
SMILES:	CCCCCCCNC
Mol. weight [g/mol]:	157.30

Physical Properties

Property code	Value	Unit	Source
gf	122.71	kJ/mol	Joback Method
hf	-196.26	kJ/mol	Joback Method
hfus	26.75	kJ/mol	Joback Method
hvap	44.29	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	2.956		Crippen Method
mcvol	161.740	ml/mol	McGowan Method
pc	2133.46	kPa	Joback Method
rinsol	1146.00		NIST Webbook
tb	478.37	K	Joback Method
tc	644.75	K	Joback Method
tf	255.12	K	Joback Method
vc	0.630	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.12	J/mol×K	478.37	Joback Method
cpg	383.54	J/mol×K	506.10	Joback Method
cpg	398.36	J/mol×K	533.83	Joback Method
cpg	412.60	J/mol×K	561.56	Joback Method
cpg	426.27	J/mol×K	589.29	Joback Method
cpg	439.38	J/mol×K	617.02	Joback Method
cpg	451.96	J/mol×K	644.75	Joback Method

Sources

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=R521607&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	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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