Phenethylamine, «alpha»-methyl-N-propyl-

Other names:	1-Phenyl-2-n-propylamino-propane
	«alpha» Phenyl-«beta» propylamino propane
	1-Phenyl-2-propylaminopropane
	N-n-Propylamphetamine
	N-Propylamphetamine
	Propylamphetamine
	26640-61-9
Inchi:	InChI=1S/C12H19N/c1-3-9-13-11(2)10-12-7-5-4-6-8-12/h4-8,11,13H,3,9-10H2,1-2H3
InchiKey:	SNPGTHLGFHVIDA-UHFFFAOYSA-N
Formula:	C12H19N
SMILES:	CCCNC(C)Cc1ccccc1
Mol. weight [g/mol]:	177.29
CAS:	51799-32-7

Physical Properties

Property code	Value	Unit	Source
gf	249.52	kJ/mol	Joback Method
hf	-6.29	kJ/mol	Joback Method
hfus	22.45	kJ/mol	Joback Method
hvap	50.63	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	2.617		Crippen Method
mcvol	166.160	ml/mol	McGowan Method
pc	2455.60	kPa	Joback Method
rinpol	1326.00		NIST Webbook
rinpol	1325.00		NIST Webbook
rinpol	1333.50		NIST Webbook
rinpol	1318.00		NIST Webbook
rinpol	1324.00		NIST Webbook
rinpol	1325.00		NIST Webbook
rinpol	1333.50		NIST Webbook
rinpol	1318.00		NIST Webbook
rinpol	1326.00		NIST Webbook
ripol	1634.00		NIST Webbook
ripol	1634.00		NIST Webbook
tb	550.37	K	Joback Method
tc	755.01	K	Joback Method

tf	289.08	K	Joback Method
vc	0.628	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.67	J/mol×K	550.37	Joback Method
cpg	415.74	J/mol×K	584.48	Joback Method
cpg	431.83	J/mol×K	618.58	Joback Method
cpg	446.99	J/mol×K	652.69	Joback Method
cpg	461.26	J/mol×K	686.80	Joback Method
cpg	474.67	J/mol×K	720.91	Joback Method
cpg	487.26	J/mol×K	755.01	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C51799327&Units=SI
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

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
ripol: Polar retention indices

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume