Pargyline

Other names:	Benzenemethanamine, N-methyl-N-2-propynyl- Benzylamine, N-methyl-N-2-propynyl- A 19120 Eudatin MO 911 N-Methyl-N-Benzylpropynylamine N-Methyl-N-propargylbenzylamine N-Methyl-N-2-propynylbenzylamine Pargylamine Pargylin Supirdyl Benzyl-methyl-2-propinylamin N-Benzyl-N-methyl-2-propynylamine Paragyline Benzylmethylpropargylamine
Inchi:	InChI=1S/C11H13N/c1-3-9-12(2)10-11-7-5-4-6-8-11/h1,4-8H,9-10H2,2H3
InchiKey:	DPWPWRLQFGFJFI-UHFFFAOYSA-N
Formula:	C11H13N
SMILES:	C#CCN(C)Cc1ccccc1
Mol. weight [g/mol]:	159.23
CAS:	555-57-7

Physical Properties

Property code	Value	Unit	Source
gf	488.00	kJ/mol	Joback Method
hf	325.59	kJ/mol	Joback Method
hfus	24.28	kJ/mol	Joback Method
hvap	44.26	kJ/mol	Joback Method
log10ws	-2.39		Crippen Method
logp	1.752		Crippen Method
mcvol	143.470	ml/mol	McGowan Method
pc	3096.73	kPa	Joback Method
rinpol	1216.00		NIST Webbook
rinpol	1227.00		NIST Webbook
rinpol	1220.00		NIST Webbook
rinpol	1215.00		NIST Webbook
rinpol	1215.00		NIST Webbook

rinpol	1232.00		NIST Webbook
rinpol	1216.00		NIST Webbook
rinpol	1215.00		NIST Webbook
rinpol	1214.00		NIST Webbook
ripol	1771.00		NIST Webbook
ripol	1762.00		NIST Webbook
ripol	1759.00		NIST Webbook
tb	480.32	K	Joback Method
tc	694.40	K	Joback Method
tf	319.59	K	Joback Method
vc	0.523	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.82	J/mol×K	480.32	Joback Method
cpg	315.45	J/mol×K	516.00	Joback Method
cpg	330.05	J/mol×K	551.68	Joback Method
cpg	343.67	J/mol×K	587.36	Joback Method
cpg	356.38	J/mol×K	623.04	Joback Method
cpg	368.23	J/mol×K	658.72	Joback Method
cpg	379.27	J/mol×K	694.40	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	360.20	K	0.50	NIST Webbook
tbrp	369.70	K	1.50	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C555577&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

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