Pentorex

Inchi:	InChI=1S/C11H17N/c1-9(11(2,3)12)10-7-5-4-6-8-10/h4-9H,12H2,1-3H3
InchiKey:	UMWAUEZOGHNSCH-UHFFFAOYSA-N
Formula:	C11H17N
SMILES:	CC(c1ccccc1)C(C)(C)N
Mol. weight [g/mol]:	163.26
CAS:	434-43-5

Physical Properties

Property code	Value	Unit	Source
gf	221.00	kJ/mol	Joback Method
hf	-14.08	kJ/mol	Joback Method
hfus	12.55	kJ/mol	Joback Method
hvap	51.31	kJ/mol	Joback Method
log10ws	-3.04		Crippen Method
logp	2.527		Crippen Method
mcvol	152.070	ml/mol	McGowan Method
pc	2893.62	kPa	Joback Method
rinpol	1261.00		NIST Webbook
rinpol	1261.00		NIST Webbook
rinpol	1256.00		NIST Webbook
rinpol	1256.00		NIST Webbook
rinpol	1256.00		NIST Webbook
ripol	1648.00		NIST Webbook
ripol	1648.00		NIST Webbook
ripol	1648.00		NIST Webbook
tb	546.62	K	Joback Method
tc	777.66	K	Joback Method
tf	310.83	K	Joback Method
vc	0.555	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	366.25	J/mol×K	546.62	Joback Method

cpg	383.56	J/mol×K	585.13	Joback Method
cpg	399.61	J/mol×K	623.63	Joback Method
cpg	414.48	J/mol×K	662.14	Joback Method
cpg	428.24	J/mol×K	700.65	Joback Method
cpg	440.98	J/mol×K	739.16	Joback Method
cpg	452.77	J/mol×K	777.66	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C434435&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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