

Benzedrex

Other names:	Cyclohexaneethanamine, N, «alpha»-dimethyl- Propylhexedrine Cyclohexaneethylamine, N-«alpha»-dimethyl- CHP-Depot Hexahydrodesoxyephedrine Hydromethamphetamine Methyl-(1-methyl-2-cyclohexylethyl)amine N, «alpha»-Dimethylcyclohexaneethylamine Obesin Obesine Propylhexadrine Propylhexedrin 1-Cyclohexyl-2-(methylamino)propane Dristan Cyclohexaneethylamine, «alpha»,N-dimethyl- 1-Cyclohexyl-2-methylaminopropan 1-Cyclohexyl-N-methyl-2-propanamine «alpha»,N-Dimethylcyclohexaneethylamine Dristan inhaler Cyclohexaneethanamine, N, «alpha»-dimethyl-, (.+/-.) (.+/-.)-N, «alpha»-Dimethylcyclohexaneethylamine N-Methyl-1-cyclohexylisopropylamine NSC 32410 N, «alpha»-dimethylcyclohexanethylamine
Inchi:	InChI=1S/C10H21N/c1-9(11-2)8-10-6-4-3-5-7-10/h9-11H,3-8H2,1-2H3
InchiKey:	JCRIVQIOJSSCQD-UHFFFAOYSA-N
Formula:	C10H21N
SMILES:	CNC(C)CC1CCCCC1
Mol. weight [g/mol]:	155.28
CAS:	101-40-6

Physical Properties

Property code	Value	Unit	Source
gf	144.72	kJ/mol	Joback Method
hf	-147.22	kJ/mol	Joback Method
hfus	15.07	kJ/mol	Joback Method

hvap	44.33		kJ/mol	Joback Method
log10ws	-2.96			Crippen Method
logp	2.565			Crippen Method
mcvol	150.880		ml/mol	McGowan Method
pc	2624.46		kPa	Joback Method
rinpol	1193.00			NIST Webbook
rinpol	1187.00			NIST Webbook
rinpol	1157.00			NIST Webbook
rinpol	1169.00			NIST Webbook
rinpol	1170.00			NIST Webbook
rinpol	1160.00			NIST Webbook
rinpol	1179.00			NIST Webbook
rinpol	1179.00			NIST Webbook
rinpol	1185.00			NIST Webbook
rinpol	1210.00			NIST Webbook
rinpol	1200.00			NIST Webbook
rinpol	1170.00			NIST Webbook
ripol	1410.00			NIST Webbook
ripol	1421.00			NIST Webbook
ripol	1431.00			NIST Webbook
tb	497.48		K	Joback Method
tc	700.99		K	Joback Method
tf	247.50		K	Joback Method
vc	0.557		m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	355.48	J/mol×K	497.48	Joback Method
cpg	375.40	J/mol×K	531.40	Joback Method
cpg	394.29	J/mol×K	565.32	Joback Method
cpg	412.17	J/mol×K	599.24	Joback Method
cpg	429.08	J/mol×K	633.15	Joback Method
cpg	445.04	J/mol×K	667.07	Joback Method
cpg	460.08	J/mol×K	700.99	Joback Method
hvapt	50.20	kJ/mol	285.00	NIST Webbook

Sources

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=C101406&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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
h vap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	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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