

3,4-Methylenedioxyphentermine

Inchi:	InChI=1S/C11H15NO2/c1-11(2,12)6-8-3-4-9-10(5-8)14-7-13-9/h3-5H,6-7,12H2,1-2H3
InchiKey:	OIZBHKBNZRXSM-UHFFFAOYSA-N
Formula:	C11H15NO2
SMILES:	CC(C)(N)Cc1ccc2c(c1)OCO2
Mol. weight [g/mol]:	193.24

Physical Properties

Property code	Value	Unit	Source
gf	100.40	kJ/mol	Joback Method
hf	-202.60	kJ/mol	Joback Method
hfus	28.31	kJ/mol	Joback Method
hvap	62.27	kJ/mol	Joback Method
log10ws	-2.87		Crippen Method
logp	1.695		Crippen Method
mcvol	152.950	ml/mol	McGowan Method
pc	3257.86	kPa	Joback Method
rinpol	1646.00		NIST Webbook
rinpol	1646.00		NIST Webbook
rinpol	1681.00		NIST Webbook
rinpol	1681.00		NIST Webbook
rinpol	1681.00		NIST Webbook
rinpol	1646.00		NIST Webbook
ripol	2379.00		NIST Webbook
ripol	2379.00		NIST Webbook
ripol	2379.00		NIST Webbook
tb	622.33	K	Joback Method
tc	861.51	K	Joback Method
tf	426.19	K	Joback Method
vc	0.561	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	408.60	J/molxK	622.33	Joback Method

cpg	423.21	J/mol×K	662.19	Joback Method
cpg	436.66	J/mol×K	702.06	Joback Method
cpg	449.08	J/mol×K	741.92	Joback Method
cpg	460.56	J/mol×K	781.78	Joback Method
cpg	471.23	J/mol×K	821.64	Joback Method
cpg	481.18	J/mol×K	861.51	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R17373&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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