

(1S,2R)-(+)-Norephedrine

Inchi:	InChI=1S/C9H13NO/c1-7(10)9(11)8-5-3-2-4-6-8/h2-7,9,11H,10H2,1H3/t7-,9-/m0/s1
InchiKey:	DLNKOYKMWOXYQA-CBAPKCEASA-N
Formula:	C9H13NO
SMILES:	CC(N)C(O)c1ccccc1
Mol. weight [g/mol]:	151.21
CAS:	37577-28-9

Physical Properties

Property code	Value	Unit	Source
gf	62.06	kJ/mol	Joback Method
hf	-121.56	kJ/mol	Joback Method
hfus	15.35	kJ/mol	Joback Method
hvap	64.45	kJ/mol	Joback Method
log10ws	-1.96		Crippen Method
logp	1.067		Crippen Method
mcvol	129.760	ml/mol	McGowan Method
pc	3975.52	kPa	Joback Method
tb	595.83	K	Joback Method
tc	808.08	K	Joback Method
tf	331.69	K	Joback Method
vc	0.468	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.04	J/mol×K	595.83	Joback Method
cpg	335.03	J/mol×K	631.21	Joback Method
cpg	346.24	J/mol×K	666.58	Joback Method
cpg	356.72	J/mol×K	701.96	Joback Method
cpg	366.49	J/mol×K	737.33	Joback Method
cpg	375.60	J/mol×K	772.71	Joback Method
cpg	384.09	J/mol×K	808.08	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C37577289&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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