

Suloctidil

Inchi:	InChI=1S/C20H35NOS/c1-5-6-7-8-9-10-15-21-17(4)20(22)18-11-13-19(14-12-18)23-16(2)
InchiKey:	BFCDFHTSVTWOG-UHFFFAOYSA-N
Formula:	C20H35NOS
SMILES:	CCCCCCCCNC(C)C(O)c1ccc(SC(C)C)cc1
Mol. weight [g/mol]:	337.56
CAS:	54063-56-8

Physical Properties

Property code	Value	Unit	Source
gf	198.67	kJ/mol	Joback Method
hf	-303.80	kJ/mol	Joback Method
hfus	43.96	kJ/mol	Joback Method
hvap	91.82	kJ/mol	Joback Method
log10ws	-6.76		Crippen Method
logp	5.559		Crippen Method
mcvol	301.100	ml/mol	McGowan Method
pc	1396.46	kPa	Joback Method
tb	898.47	K	Joback Method
tc	1106.19	K	Joback Method
tf	456.98	K	Joback Method
vc	1.137	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	969.18	J/molxK	898.47	Joback Method
cpg	985.30	J/molxK	933.09	Joback Method
cpg	1000.31	J/molxK	967.71	Joback Method
cpg	1014.25	J/molxK	1002.33	Joback Method
cpg	1027.19	J/molxK	1036.95	Joback Method
cpg	1039.19	J/molxK	1071.57	Joback Method
cpg	1050.28	J/molxK	1106.19	Joback Method

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=C54063568&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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