Nortropan-3«beta»-ol

Inchi: InChI=1S/C7H13NO/c9-7-3-5-1-2-6(4-7)8-5/h5-9H,1-4H2/t5-,6+,7-
InchiKey: YYMCYJLIYNNOMK-KVSKUHBBSA-N
Formula: C7H13NO
SMILES: OC1CC2CCC(C1)N2
Mol. weight [g/mol]: 127.18

Physical Properties

Property code	Value	Unit	Source
gf	48.54	kJ/mol	Joback Method
hf	-189.29	kJ/mol	Joback Method
hfus	20.71	kJ/mol	Joback Method
hvap	54.47	kJ/mol	Joback Method
log10ws	-1.33		Crippen Method
logp	0.262		Crippen Method
mcvol	103.620	ml/mol	McGowan Method
pc	4468.24	kPa	Joback Method
rinpol	1160.00		NIST Webbook
rinpol	1160.00		NIST Webbook
tb	517.64	K	Joback Method
tc	723.80	K	Joback Method
tf	359.10	K	Joback Method
vc	0.381	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	259.65	J/mol×K	517.64	Joback Method
cpg	274.10	J/mol×K	552.00	Joback Method
cpg	287.71	J/mol×K	586.36	Joback Method
cpg	300.51	J/mol×K	620.72	Joback Method
cpg	312.56	J/mol×K	655.08	Joback Method
cpg	323.89	J/mol×K	689.44	Joback Method
cpg	334.53	J/mol×K	723.80	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R510162&Units=SI

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