3«beta»-n-Butyroxynortropane

Inchi: InChI=1S/C11H19NO2/c1-2-3-11(13)14-10-6-8-4-5-9(7-10)12-8/h8-10,12H,2-7H2,1H3/t8
InchiKey: NXBJEYZOFCMPDB-ILWJIGKKSA-N
Formula: C11H19NO2
SMILES: CCCC(=O)OC1CC2CCC(C1)N2
Mol. weight [g/mol]: 197.27

Physical Properties

Property code	Value	Unit	Source
gf	-14.88	kJ/mol	Joback Method
hf	-364.42	kJ/mol	Joback Method
hfus	29.76	kJ/mol	Joback Method
hvap	55.86	kJ/mol	Joback Method
log10ws	-2.60		Crippen Method
logp	1.613		Crippen Method
mcvol	161.550	ml/mol	McGowan Method
pc	2695.80	kPa	Joback Method
rinpol	1440.00		NIST Webbook
rinpol	1440.00		NIST Webbook
tb	593.27	K	Joback Method
tc	807.28	K	Joback Method
tf	415.52	K	Joback Method
vc	0.610	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	439.78	J/mol×K	593.27	Joback Method
cpg	458.44	J/mol×K	628.94	Joback Method
cpg	476.02	J/mol×K	664.61	Joback Method
cpg	492.56	J/mol×K	700.28	Joback Method
cpg	508.09	J/mol×K	735.95	Joback Method
cpg	522.64	J/mol×K	771.62	Joback Method
cpg	536.27	J/mol×K	807.28	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=R509701&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