

6-Butyroxynortropan-3-ol

Inchi:	InChI=1S/C11H19NO3/c1-2-3-11(14)15-10-5-7-4-8(13)6-9(10)12-7/h7-10,12-13H,2-6H2,
InchiKey:	XYVUORHYOWDSSK-QGVKSAJWSA-N
Formula:	C11H19NO3
SMILES:	CCCC(=O)OC1CC2CC(O)CC1N2
Mol. weight [g/mol]:	213.27

Physical Properties

Property code	Value	Unit	Source
gf	-159.41	kJ/mol	Joback Method
hf	-536.99	kJ/mol	Joback Method
hfus	34.92	kJ/mol	Joback Method
hvap	72.23	kJ/mol	Joback Method
log10ws	-1.98		Crippen Method
logp	0.584		Crippen Method
mcvol	167.420	ml/mol	McGowan Method
pc	2868.87	kPa	Joback Method
rinpol	1632.00		NIST Webbook
tb	680.78	K	Joback Method
tc	880.99	K	Joback Method
tf	472.10	K	Joback Method
vc	0.627	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	505.76	J/molxK	680.78	Joback Method
cpg	521.35	J/molxK	714.15	Joback Method
cpg	536.03	J/molxK	747.52	Joback Method
cpg	549.84	J/molxK	780.88	Joback Method
cpg	562.80	J/molxK	814.25	Joback Method
cpg	574.94	J/molxK	847.62	Joback Method
cpg	586.27	J/molxK	880.99	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=R509929&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
mccvol:	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

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