Butacaine

Other names:	1-Propanol, 3-(dibutylamino)-, 4-aminobenzoate (ester) 1-Propanol, 3-(dibutylamino)-, p-aminobenzoate (ester) p-Aminobenzoyldibutylaminopropanol Butelline Butyn 3-(Dibutylamino)-1-propanol p-aminobenzoate 3-Dibutylaminopropyl p-aminobenzoate 1-Propanol, 3-(dibutylamino)-, 4-aminobenzoate 1-Propanol, 3-(dibutylamino)-, p-aminobenzoate 3-(p-Aminobenzoxy)-1-di-n-butylaminopropane (3-di-N-Butylaminopropyl)-p-aminobenzoate (3'-Di-n-butylaminopropyl)-p-aminobenzoate
Inchi:	InChI=1S/C18H30N2O2/c1-3-5-12-20(13-6-4-2)14-7-15-22-18(21)16-8-10-17(19)11-9-16
InchiKey:	HQFWVSGBVLEQGA-UHFFFAOYSA-N
Formula:	C18H30N2O2
SMILES:	CCCCN(CCCC)CCCOC(=O)c1ccc(N)cc1
Mol. weight [g/mol]:	306.44
CAS:	149-16-6

Physical Properties

Property code	Value	Unit	Source
gf	146.77	kJ/mol	Joback Method
hf	-333.27	kJ/mol	Joback Method
hfus	47.03	kJ/mol	Joback Method
hvap	80.44	kJ/mol	Joback Method
log10ws	-4.10		Crippen Method
logp	3.718		Crippen Method
mcvol	268.120	ml/mol	McGowan Method
pc	1563.52	kPa	Joback Method
rinpol	2445.00		NIST Webbook
rinpol	2436.00		NIST Webbook
rinpol	2436.00		NIST Webbook
rinpol	2422.00		NIST Webbook
rinpol	2450.00		NIST Webbook
rinpol	2457.00		NIST Webbook
rinpol	2457.00		NIST Webbook
rinpol	2436.00		NIST Webbook

rinpol	2471.00		NIST Webbook
ripol	3646.00		NIST Webbook
tb	804.16	K	Joback Method
tc	1004.29	K	Joback Method
tf	519.45	K	Joback Method
vc	1.006	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	824.74	J/mol×K	804.16	Joback Method
cpg	841.34	J/mol×K	837.51	Joback Method
cpg	856.89	J/mol×K	870.87	Joback Method
cpg	871.42	J/mol×K	904.22	Joback Method
cpg	884.99	J/mol×K	937.58	Joback Method
cpg	897.63	J/mol×K	970.93	Joback Method
cpg	909.38	J/mol×K	1004.29	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C149166&Units=SI
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

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