

AMBUCETAMIDE

Other names:	Benzeneacetamide, «alpha»-(dibutylamino)-4-methoxy-Acetamide, 2-dibutylamino-2-(p-methoxyphenyl)-A 16 Ambucetamid «alpha»-Dibutylamino-«alpha»-(p-methoxyphenyl)acetamide Bersen Dibutamid Dibutamide «alpha»-Dibutyl-amino-4-methoxybenzeneacetamide «alpha»-Dibutyl-amino-p-methoxyphenylacetamide 2-Dibutylamino-2-(p-methoxyphenyl)acetamide Meritin «alpha»-p-Methoxyphenyl-«alpha»-di-n-butylaminoacetamide R 5 (.+/-.)-Ambucetamide
Inchi:	InChI=1S/C17H28N2O2/c1-4-6-12-19(13-7-5-2)16(17(18)20)14-8-10-15(21-3)11-9-14/h8
InchiKey:	WUSAVCGXMSWMQM-UHFFFAOYSA-N
Formula:	C17H28N2O2
SMILES:	CCCCN(CCCC)C(C(N)=O)c1ccc(OC)cc1
Mol. weight [g/mol]:	292.42

Physical Properties

Property code	Value	Unit	Source
hfus	40.92	kJ/mol	Joback Method
ie	6.92	eV	Cheméo Relay (1.0)
logp	3.124		Crippen Method
mcvol	254.030	ml/mol	McGowan Method
rinpol	2235.00		NIST Webbook
tb	621.65	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	767.48	J/mol×K	780.84	Joback Method

cpg	784.05	J/mol×K	814.73	Joback Method
cpg	799.56	J/mol×K	848.62	Joback Method
cpg	814.04	J/mol×K	882.51	Joback Method
cpg	827.53	J/mol×K	916.40	Joback Method
cpg	840.08	J/mol×K	950.28	Joback Method
cpg	851.73	J/mol×K	984.17	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C519880&Units=SI>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

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
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature

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