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
CAS:	519-88-0

Physical Properties

Property code	Value	Unit	Source
gf	135.91	kJ/mol	Joback Method
hf	-317.91	kJ/mol	Joback Method
hfus	40.92	kJ/mol	Joback Method
hvap	77.83	kJ/mol	Joback Method
log10ws	-3.98		Crippen Method
logp	3.124		Crippen Method
mcvol	254.030	ml/mol	McGowan Method
pc	1700.50	kPa	Joback Method
rinpol	2235.00		NIST Webbook
tb	780.84	K	Joback Method
tc	984.17	K	Joback Method
tf	493.18	K	Joback Method
vc	0.945	m3/kmol	Joback Method

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

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=C519880&Units=SI
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
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