

Metabutoxycaine

Inchi:	InChI=1S/C17H28N2O3/c1-4-7-12-21-16-14(9-8-10-15(16)18)17(20)22-13-11-19(5-2)6-3
InchiKey:	LJQWYEFHNLTPBZ-UHFFFAOYSA-N
Formula:	C17H28N2O3
SMILES:	CCCCOc1c(N)cccc1C(=O)OCCN(CC)CC
Mol. weight [g/mol]:	308.42
CAS:	3624-87-1

Physical Properties

Property code	Value	Unit	Source
gf	23.72	kJ/mol	Joback Method
hf	-456.32	kJ/mol	Joback Method
hfus	45.24	kJ/mol	Joback Method
hvap	81.29	kJ/mol	Joback Method
log10ws	-3.39		Crippen Method
logp	2.946		Crippen Method
mvol	259.900	ml/mol	McGowan Method
pc	1645.76	kPa	Joback Method
rinpol	2226.00		NIST Webbook
rinpol	2226.00		NIST Webbook
tb	808.68	K	Joback Method
tc	1010.19	K	Joback Method
tf	542.93	K	Joback Method
vc	0.969	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	795.30	J/molxK	808.68	Joback Method
cpg	811.15	J/molxK	842.26	Joback Method
cpg	825.94	J/molxK	875.85	Joback Method
cpg	839.69	J/molxK	909.43	Joback Method
cpg	852.43	J/molxK	943.02	Joback Method
cpg	864.18	J/molxK	976.60	Joback Method
cpg	874.95	J/molxK	1010.19	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3624871&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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