

Tetracaine

Other names:

2-(Dimethylamino)ethyl p-(butylamino)benzoate
2-Dimethylaminoethylester kyseliny p-butylaminobenzoove
Amethocaine
Anetain
Benzoic acid, 4-(butylamino)-, 2-(dimethylamino)ethyl ester
Benzoic acid, p-(butylamino)-, 2-(dimethylamino)ethyl ester
Butylocaine
Contralgin
Diaethylaminoaethanol ester der p-butylaminobenzoesaere
Dicain
Dicaine
Dikain
Dimethylaminoethyl p-butyl-aminobenzoate
Fissucain
Intercain
Landocaine
Laudocaine
Medicaine
Medihaler-tetracaine
Meethobalm
Metraspray
Mucaesthin
Niphanoid
Pontocaine
Rexocaine
Tetrakain
Uromucaesthin
p-(Butylamino)benzoic acid, 2-(dimethylamino)ethyl ester

«beta»-Dimethylaminoethyl p-butylaminobenzoate
Â«betaÂ»-Dimethylaminoethyl p-butylaminobenzoate

Inchi: InChI=1S/C15H24N2O2/c1-4-5-10-16-14-8-6-13(7-9-14)15(18)19-12-11-17(2)3/h6-9,16H

InchiKey: GKCB AIGFKIBETG-UHFFFAOYSA-N

Formula: C15H24N2O2

SMILES: CCCCNc1ccc(C(=O)OCCN(C)C)cc1

Mol. weight [g/mol]: 264.36

CAS: 94-24-6

Physical Properties

Property code	Value	Unit	Source
gf	144.45	kJ/mol	Joback Method
hf	-251.67	kJ/mol	Joback Method
h _{fus}	39.16	kJ/mol	Joback Method
h _{vap}	69.56	kJ/mol	Joback Method
log ₁₀ ws	-3.01		Aqueous Solubility Prediction Method
logp	2.617		Crippen Method
m _{cvol}	225.850	ml/mol	McGowan Method
pc	1915.26	kPa	Joback Method
rinpol	2224.00		NIST Webbook
rinpol	2235.00		NIST Webbook
rinpol	2197.00		NIST Webbook
rinpol	2219.00		NIST Webbook
rinpol	2224.00		NIST Webbook
rinpol	2230.00		NIST Webbook
rinpol	2219.00		NIST Webbook
rinpol	2215.00		NIST Webbook
rinpol	2212.00		NIST Webbook
rinpol	2212.00		NIST Webbook
rinpol	2221.00		NIST Webbook
rinpol	2218.00		NIST Webbook
rinpol	2229.00		NIST Webbook
tb	713.16	K	Joback Method
tc	910.48	K	Joback Method
tf	455.04	K	Joback Method
vc	0.845	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	642.99	J/mol×K	713.16	Joback Method
cpg	659.18	J/mol×K	746.05	Joback Method
cpg	674.41	J/mol×K	778.93	Joback Method
cpg	688.70	J/mol×K	811.82	Joback Method
cpg	702.08	J/mol×K	844.71	Joback Method
cpg	714.60	J/mol×K	877.59	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C94246&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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