

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 | 2219.00 | | NIST Webbook |
| rinpol | 2230.00 | | NIST Webbook |
| rinpol | 2197.00 | | NIST Webbook |
| rinpol | 2219.00 | | NIST Webbook |
| rinpol | 2212.00 | | NIST Webbook |
| rinpol | 2212.00 | | NIST Webbook |
| rinpol | 2221.00 | | NIST Webbook |
| rinpol | 2215.00 | | NIST Webbook |
| rinpol | 2218.00 | | NIST Webbook |
| rinpol | 2229.00 | | NIST Webbook |
| rinpol | 2235.00 | | NIST Webbook |
| rinpol | 2224.00 | | NIST Webbook |
| rinpol | 2224.00 | | 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 |
| 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 |

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