

Benzenepropanaminium, «gamma»-(aminocarbonyl)-N-methyl-N,N-bis(1-m

Other names:

Ammonium, (3-carbamoyl-3,3-diphenylpropyl)diisopropylmethyl-

(3-Carbamoyl-3,3-diphenylpropyl)diisopropylmethylammonium

Isopropamid

Isopropamide

Isopropanamide

(3-Carbamoyl-3,3-diphenylpropyl)diisopropylmethylamine

Inchi: InChI=1S/C22H30N2O/c1-17(2)24(18(3)4)16-15-22(21(23)25,19-11-7-5-8-12-19)20-13-9

InchiKey: KNIVGGRCJWRCDV-UHFFFAOYSA-N

Formula: C23H33N2O

SMILES: CC(C)N(CCC(C(N)=O)(c1ccccc1)c1ccccc1)C(C)C

Mol. weight [g/mol]: 353.52

CAS: 7492-32-2

Physical Properties

Property code	Value	Unit	Source
gf	405.45	kJ/mol	Joback Method
hf	-54.92	kJ/mol	Joback Method
hfus	36.18	kJ/mol	Joback Method
hvap	86.48	kJ/mol	Joback Method
log10ws	-5.02		Crippen Method
logp	3.967		Crippen Method
mcvol	294.850	ml/mol	McGowan Method
pc	1580.97	kPa	Joback Method
tb	890.85	K	Joback Method
tc	1125.49	K	Joback Method
tf	528.62	K	Joback Method
vc	1.081	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	938.68	J/mol×K	890.85	Joback Method
cpg	955.57	J/mol×K	929.96	Joback Method
cpg	971.23	J/mol×K	969.06	Joback Method

cpg	985.80	J/mol×K	1008.17	Joback Method
cpg	999.45	J/mol×K	1047.27	Joback Method
cpg	1012.31	J/mol×K	1086.38	Joback Method
cpg	1024.53	J/mol×K	1125.49	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7492322&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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