ISOPROPAMIDE

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:	C22H30N2O
SMILES:	CC(C)N(CCC(C(N)=O)(c1ccccc1)c1ccccc1)C(C)C
Mol. weight [g/mol]:	338.49

Physical Properties

Property code	Value	Unit	Source
hfus	36.18	kJ/mol	Joback Method
log10ws	-3.07		Cheméo Relay (1.0)
logp	3.967		Crippen Method
mcvol	294.850	ml/mol	McGowan Method
tf	387.57	K	Cheméo Relay (1.0)

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

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7492322&Units=SI
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
hfus:	Enthalpy of fusion at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point