

Acetamide, 2,2-diphenyl-2-(2-(N-methyl-N-isopropylamino)ethyl) (decomposition product of Isopropamide)

InChI: InChI=1S/C20H26N2O/c1-16(2)27(3)15-14-20(19(21)23-17-10-6-7-11-17)18-12-8-5-9-
InChIKey: KUQRRPX1MLQWRE-UHFFFAOYSA-N

Formula: C20H26N2O

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

Mol. weight [g/mol]: 310.43

Physical Properties

Property code	Value	Unit	Source
gf	391.05	kJ/mol	Joback Method
hf	-8.36	kJ/mol	Joback Method
hfus	34.52	kJ/mol	Joback Method
hvap	82.41	kJ/mol	Joback Method
log10ws	-4.07		Crippen Method
logp	3.188		Crippen Method
mcvol	266.670	ml/mol	McGowan Method
pc	1840.41	kPa	Joback Method
rinpol	2679.00		NIST Webbook
tb	845.53	K	Joback Method
tc	1082.77	K	Joback Method
tf	521.08	K	Joback Method
vc	0.976	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	821.21	J/molxK	845.53	Joback Method
cpg	837.75	J/molxK	885.07	Joback Method
cpg	853.02	J/molxK	924.61	Joback Method
cpg	867.16	J/molxK	964.15	Joback Method
cpg	880.31	J/molxK	1003.69	Joback Method
cpg	892.62	J/molxK	1043.23	Joback Method
cpg	904.24	J/molxK	1082.77	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R490954&Units=SI

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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