Benzamide, N-(1-methylethyl)-4-[(2-methylhydrazino)methyl]-

Other names: p-Toluamide, N-isopropyl-«alpha»-(2-methylhydrazino)-
Ibenzmethyzine
2-(p-Isopropylcarbamoylbenzyl)-1-methylhydrazine
N-Isopropyl-«alpha»-(2-methylhydrazino)-p-toluamide
4-((2-Methylhydrazino)methyl)-N-isopropylbenzamide
1-Methyl-2-(p-(isopropylcarbamoyl)benzyl)hydrazine
MIH
Natulan
NSC-77213
PCB
Procarbazin
Procarbazine
RO 4-6467
N-(1-Methylethyl)-4-[(2-methylhydrazino)methyl]benzamide
CB 400-497
p-(2-Methylhydrazinomethyl)-N-isopropylbenzamide

Inchi: InChI=1S/C12H19N3O/c1-9(2)15-12(16)11-6-4-10(5-7-11)8-14-13-3/h4-7,9,13-14H,8H2,

InchiKey: CPTBDICYNRMXFX-UHFFFAOYSA-N

Formula: C12H19N3O

SMILES: CNNCc1ccc(C(=O)NC(C)C)cc1

Mol. weight [g/mol]: 221.30

CAS: 671-16-9

Physical Properties

Property code	Value	Unit	Source
gf	289.75	kJ/mol	Joback Method
hf	-23.40	kJ/mol	Joback Method
hfus	33.86	kJ/mol	Joback Method
hvap	70.91	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	1.049		Crippen Method
mcvol	187.690	ml/mol	McGowan Method
pc	2646.11	kPa	Joback Method
rinpol	1975.00		NIST Webbook
rinpol	1990.00		NIST Webbook
tb	709.56	K	Joback Method
tc	921.85	K	Joback Method

tf	456.85	K	Joback Method
vc	0.705	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	525.21	J/mol×K	709.56	Joback Method
cpg	539.51	J/mol×K	744.94	Joback Method
cpg	552.87	J/mol×K	780.32	Joback Method
cpg	565.32	J/mol×K	815.70	Joback Method
cpg	576.90	J/mol×K	851.08	Joback Method
cpg	587.66	J/mol×K	886.46	Joback Method
cpg	597.63	J/mol×K	921.85	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=C671169&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
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