PROCARBAZINE

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

Physical Properties

Property code	Value	Unit	Source
hfus	33.86	kJ/mol	Joback Method
logp	1.049		Crippen Method
mcvol	187.690	ml/mol	McGowan Method
rinpol	1990.00		NIST Webbook
rinpol	1975.00		NIST Webbook
rinpol	2000.00		NIST Webbook
rinpol	1990.00		NIST Webbook
rinpol	1990.00		NIST Webbook
rinpol	1975.00		NIST Webbook

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

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C671169&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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):

Legend

cpg: Ideal gas heat capacity

hfus: Enthalpy of fusion at standard conditions

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices