1-(2-ISOPROPYL-4-PENTENOYL)UREA

Other names:	(2-Isopropyl-4-pentenoyl)urea
	(2-isopropylpent-4-enoyl)urea
	(Allylisopropylacetyl)carbamide
	(Allylisopropylacetyl)urea
	4-Pentenamide, N-(aminocarbonyl)-2-(1-methylethyl)-
	Apronal
	Apronalide
	Isodormid
	Isopropylallylazetylkarbamid
	N-(Aminocarbonyl)-2-(1-methylethyl)-4-pentenamide
	N-carbamoyl-2-propan-2-ylpent-4-enamide
	Sedormid
Inchi:	InChI=1S/C9H16N2O2/c1-4-5-7(6(2)3)8(12)11-9(10)13/h4,6-7H,1,5H2,2-3H3,(H3,10,11,1
InchiKey:	KSUUMAWCGDNLFK-UHFFFAOYSA-N
Formula:	C9H16N2O2
SMILES:	C=CCC(C(=O)NC(N)=O)C(C)C
Mol. weight [g/mol]:	184.24

Physical Properties

Property code	Value	Unit	Source
hfus	24.23	kJ/mol	Joback Method
log10ws	-2.75		Aqueous Solubility Prediction Method
logp	1.030		Crippen Method
mcvol	156.470	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	407.33	J/mol×K	631.56	Joback Method
cpg	419.82	J/mol×K	665.72	Joback Method
cpg	431.57	J/mol×K	699.87	Joback Method
cpg	442.60	J/mol×K	734.03	Joback Method
cpg	452.94	J/mol×K	768.19	Joback Method

cpg	462.63	J/mol×K	802.34	Joback Method
cpg	471.68	J/mol×K	836.50	Joback Method

Sources

Cheméo Relay (1.0, beta):

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C528927&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

Cheméo Relay (1.0):

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