Bromisovalum

Other names:

Butanamide, N-(aminocarbonyl)-2-bromo-3-methyl-
Urea, (2-bromo-3-methylbutyryl)-
«alpha»-Bromisovalerylurea
«alpha»-Bromoisovaleric acid ureide
(«alpha»-Bromo-.beta,beta.-dimethylpropanoyl)urea
(«alpha»-Bromoisovaleroyl)urea
(«alpha»-Bromoisovaleryl)urea
Abroval
Alluval
Alural
Bromaral
Bromcarbamide
Bromisoval
Bromisovalerylurea
Bromizoval
Bromocarbamide
Bromoisovalum
Bromoval
Bromovalerocarbamide
Bromovaleroylurea
Bromovalerylurea
Bromoxil
Bromural
Bromvalerylurea
Bromvaletone
Bromvalurea
Bromyl
Brovalin
Brovalurea
Brovarin
BVU
Calmotin
Dagrabromyl
Dibroluur
Dormigene
Isobromyl
Pivadorm
Pivadorn
Upiol
Uvaleral

	2-Bromo-3-Methylbutyrylurea
	2-Bromo-isovaleryl urea
	N-(Aminocarbonyl)-2-bromo-3-methylbutanamide
	2-Bromisovalerylmocovina
	Bromuvan
	Bromvaletonum
	Monobromoisovalerylurea
	2-Monobromoisovalerylurea
	Somnurol
	B.V.U.
	(.+/-.)-Bromisoval
	(RS)-2-Bromoisovalerylurea
Inchi:	InChI=1S/C6H11BrN2O2/c1-3(2)4(7)5(10)9-6(8)11/h3-4H,1-2H3,(H3,8,9,10,11)
InchiKey:	CMCCHHWTTBEZNM-UHFFFAOYSA-N
Formula:	C6H11BrN2O2
SMILES:	CC(C)C(Br)C(=O)NC(N)=O
Mol. weight [g/mol]:	223.07
CAS:	496-67-3

Physical Properties

Property code	Value	Unit	Source
gf	-92.92	kJ/mol	Joback Method
hf	-289.30	kJ/mol	Joback Method
hfus	23.03	kJ/mol	Joback Method
hvap	65.18	kJ/mol	Joback Method
log10ws	-1.79		Crippen Method
logp	0.601		Crippen Method
mcvol	136.000	ml/mol	McGowan Method
pc	4368.40	kPa	Joback Method
rinpol	1510.00		NIST Webbook
tb	632.40	K	Joback Method
tc	855.40	K	Joback Method
tf	422.96	K	Joback Method
vc	0.497	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	319.19	J/mol×K	632.40	Joback Method
cpg	328.95	J/mol×K	669.57	Joback Method
cpg	338.04	J/mol×K	706.73	Joback Method
cpg	346.50	J/mol×K	743.90	Joback Method
cpg	354.36	J/mol×K	781.07	Joback Method
cpg	361.63	J/mol×K	818.24	Joback Method
cpg	368.37	J/mol×K	855.40	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C496673&Units=SI
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

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

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