

Carbromal

Other names:

(2-Bromo-2-ethylbutyryl)urea
(«alpha»-Bromo-«alpha»-ethylbutyryl)carbamide
(«alpha»-Bromo-«alpha»-ethylbutyryl)urea
(«alpha»-Ethyl-«alpha»-bromobutyryl)urea
(Â«alphaÂ»-Bromo-Â«alphaÂ»-ethylbutyryl)carbamide
(Â«alphaÂ»-Bromo-Â«alphaÂ»-ethylbutyryl)urea
(Â«alphaÂ»-Ethyl-Â«alphaÂ»-bromobutyryl)urea
1-Bromo-ethyl-butyl-urea
2-Brom-2-ethylbutyrylmocovina
2-bromo-N-carbamoyl-2-ethylbutanamide
Adalin
Addisomnol
Adisomnol
Bromacetocarbamide
Bromadal
Bromadel
Bromdiethylacetylurea
Bromodiacetylurea
Bromodiethylacetylcarbamide
Bromodiethylacetylurea
Butanamide, N-(aminocarbonyl)-2-bromo-2-ethyl-
Diacid
Dormiturin
Fydalin
Hoggar
Karbromal
Kartryl
N-(Aminocarbonyl)-2-bromo-2-ethylbutanamide
NCI-C03805
NSC 49191
Nenesin
Nyctal
Parkosed
Pelidorm
Pianadalin
Planadalin
Tildin
Uradal
Urea, (2-bromo-2-ethylbutyryl)-

Inchi: InChI=1S/C7H13BrN2O2/c1-3-7(8,4-2)5(11)10-6(9)12/h3-4H2,1-2H3,(H3,9,10,11,12)

InchiKey: OPNPQXLQERQBBV-UHFFFAOYSA-N
Formula: C7H13BrN2O2
SMILES: CCC(Br)(CC)C(=O)NC(N)=O
Mol. weight [g/mol]: 237.09
CAS: 77-65-6

Physical Properties

Property code	Value	Unit	Source
gf	-76.78	kJ/mol	Joback Method
hf	-308.13	kJ/mol	Joback Method
hfus	25.25	kJ/mol	Joback Method
hvap	66.88	kJ/mol	Joback Method
log10ws	-2.68		Aqueous Solubility Prediction Method
log10ws	-2.68		Estimated Solubility Method
logp	1.135		Crippen Method
mcvol	150.090	ml/mol	McGowan Method
pc	3877.12	kPa	Joback Method
rinpol	1515.00		NIST Webbook
rinpol	1560.00		NIST Webbook
rinpol	1515.00		NIST Webbook
rinpol	1525.00		NIST Webbook
rinpol	1500.00		NIST Webbook
rinpol	1500.00		NIST Webbook
rinpol	1515.00		NIST Webbook
rinpol	1500.00		NIST Webbook
rinpol	1515.00		NIST Webbook
rinpol	1509.00		NIST Webbook
rinpol	1513.00		NIST Webbook
rinpol	1501.00		NIST Webbook
rinpol	1501.00		NIST Webbook
rinpol	1560.00		NIST Webbook
rinpol	1513.00		NIST Webbook
rinpol	1513.00		NIST Webbook
tb	652.93	K	Joback Method
tc	875.62	K	Joback Method
tf	466.65	K	Joback Method
vc	0.554	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	369.01	J/molxK	652.93	Joback Method
cpg	379.44	J/molxK	690.04	Joback Method
cpg	389.11	J/molxK	727.16	Joback Method
cpg	398.06	J/molxK	764.27	Joback Method
cpg	406.36	J/molxK	801.39	Joback Method
cpg	414.05	J/molxK	838.50	Joback Method
cpg	421.20	J/molxK	875.62	Joback Method

Sources

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

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

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C77656&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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
rinpolar:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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