Acetylcarbromal

Other names:	Butanamide, N-[(acetylamino)carbonyl]-2-bromo-2-ethyl-
	Acecarbromal
	Urea, 1-acetyl-3-(2-bromo-2-ethylbutyryl)-
	Abasin
	Absin
	Acetcarbromal
	Acetyl Adalin
	Adityl
	Carbased
	Darolon
	N-Acetyl-N'-diethylbromoacetylurea
	Sedamyl
	Acetylbromodiethylacetylcarbamide
	Acetkarbromal
	N-Acetyl-N'-«alpha»-bromo-«alpha»-ethylbutyrylcarbamide
	N-((Acetylamino)carbonyl)-2-bromo-2-ethylbutanamide
	1-Acetyl-3-(«alpha»-bromo-«alpha»-ethylbutyryl)urea
	1-Acetyl-3-(2-bromo-2-ethylbutyryl)urea
	Ibatran
	Paxarel
	Sedmynol
	Sedtran
Inchi:	InChI=1S/C9H15BrN2O3/c1-4-9(10,5-2)7(14)12-8(15)11-6(3)13/h4-5H2,1-3H3,(H2,11,12
InchiKey:	SAZUGELZHZOXHB-UHFFFAOYSA-N
Formula:	C9H15BrN2O3
SMILES:	CCC(Br)(CC)C(=O)NC(=O)NC(C)=O
Mol. weight [g/mol]:	279.13
CAS:	77-66-7

Physical Properties

Property code	Value	Unit	Source
gf	-165.92	kJ/mol	Joback Method
hf	-442.31	kJ/mol	Joback Method
hfus	31.93	kJ/mol	Joback Method
hvap	73.88	kJ/mol	Joback Method
log10ws	-2.82		Crippen Method

logp	1.312		Crippen Method
mcvol	179.840	ml/mol	McGowan Method
pc	3159.72	kPa	Joback Method
tb	730.20	K	Joback Method
tc	944.68	K	Joback Method
tf	508.52	K	Joback Method
vc	0.678	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	471.20	J/mol×K	730.20	Joback Method
cpg	481.84	J/mol×K	765.95	Joback Method
cpg	491.72	J/mol×K	801.69	Joback Method
cpg	500.88	J/mol×K	837.44	Joback Method
cpg	509.38	J/mol×K	873.19	Joback Method
cpg	517.28	J/mol×K	908.94	Joback Method
cpg	524.62	J/mol×K	944.68	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C77667&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume