Butanamide, 2-bromo-2-ethyl-

Other names:	Butyramide, 2-bromo-2-ethyl-
	Carabromide
	Carbromide
	Diethylbromoacetamide
	Neuronal
	2-Bromo-2-ethylbutyramide
	2-Bromo-2,2-diethylacetamide
	2-Ethyl-2-bromobutyramide
	2-Bromo-2-ethylbutanamide
	2-Bromo-2-ethylbutylamide
	NSC 4607
Inchi:	InChI=1S/C6H12BrNO/c1-3-6(7,4-2)5(8)9/h3-4H2,1-2H3,(H2,8,9)
InchiKey:	ACEYAMOAGUDVAQ-UHFFFAOYSA-N
Formula:	C6H12BrNO
SMILES:	CCC(Br)(CC)C(=N)O
Mol. weight [g/mol]:	194.07
CAS:	511-70-6

Physical Properties

Property code	Value	Unit	Source
gf	83.58	kJ/mol	Joback Method
hf	-103.49	kJ/mol	Joback Method
hvap	62.85	kJ/mol	Joback Method
log10ws	-3.61		Crippen Method
logp	2.475		Crippen Method
mcvol	124.450	ml/mol	McGowan Method
rinpol	1215.00		NIST Webbook
rinpol	1192.00		NIST Webbook
rinpol	1215.00		NIST Webbook
rinpol	1215.00		NIST Webbook
rinpol	1192.00		NIST Webbook
rinpol	1205.00		NIST Webbook
tb	576.13	K	Joback Method
tf	349.20	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.39	J/mol×K	576.13	Joback Method
cpg	46.33	J/mol×K	100.12	Joback Method
cpg	46.33	J/mol×K	100.12	Joback Method
cpg	46.33	J/mol×K	100.12	Joback Method
cpg	46.33	J/mol×K	100.12	Joback Method
cpg	46.33	J/mol×K	100.12	Joback Method
cpg	46.33	J/mol×K	100.12	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C511706&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation 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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point

Latest version available from:
https://www.chemeo.com/cid/98-490-0/Butanamide-2-bromo-2-ethyl.pdf
Generated by Cheméo on 2024-05-03 04:20:03.827110008 +0000 UTC m=+16999252.747687319.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.