

«alpha»-Bromo-«gamma»-valerolactone

Other names:	Valeric acid, 2-bromo-4-hydroxy-, «gamma»-lactone 2(3H)-Furanone, 3-bromodihydro-5-methyl- 3-Bromo-5-methyldihydro-2(3H)-furanone alpha-Bromo-gamma-valerolactone NSC 91486 alpha-bromo-«gamma»-valerolactone Alpha-bromo-gamma-valerolactone,c&t
Inchi:	InChI=1S/C5H7BrO2/c1-3-2-4(6)5(7)8-3/h3-4H,2H2,1H3
InchiKey:	FLOKBGAYTGLYGR-UHFFFAOYSA-N
Formula:	C5H7BrO2
SMILES:	CC1CC(Br)C(=O)O1
Mol. weight [g/mol]:	179.01
CAS:	25966-39-6

Physical Properties

Property code	Value	Unit	Source
gf	-174.33	kJ/mol	Joback Method
hf	-349.76	kJ/mol	Joback Method
hfus	16.49	kJ/mol	Joback Method
hvap	41.86	kJ/mol	Joback Method
log10ws	-1.33		Crippen Method
logp	1.085		Crippen Method
mcvol	95.390	ml/mol	McGowan Method
pc	4717.12	kPa	Joback Method
tb	485.34	K	Joback Method
tc	723.85	K	Joback Method
tf	307.36	K	Joback Method
vc	0.345	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	189.89	J/molxK	485.34	Joback Method
cpg	201.60	J/molxK	525.09	Joback Method

cpg	212.74	J/mol×K	564.84	Joback Method
cpg	223.30	J/mol×K	604.59	Joback Method
cpg	233.29	J/mol×K	644.35	Joback Method
cpg	242.68	J/mol×K	684.10	Joback Method
cpg	251.47	J/mol×K	723.85	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	408.00	K	1.60	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C25966396&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/30-982-8/alpha-Bromo-gamma-valerolactone.pdf>

Generated by Cheméo on 2024-05-04 17:33:48.747764301 +0000 UTC m=+17133277.668341612.

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