«gamma»-(4-Fluorophenyl)-«gamma»-butyrolacto

Other names: «gamma»-(4-Fluorophenyl)-butyrolactone
2(3H)-Furanone, 5-(4-fluorophenyl)dihydro-
Inchi: InChI=1S/C10H9FO2/c11-8-3-1-7(2-4-8)9-5-6-10(12)13-9/h1-4,9H,5-6H2
InchiKey: RMFNZGXVLAUJHF-UHFFFAOYSA-N
Formula: C10H9FO2
SMILES: O=C1CCC(c2ccc(F)cc2)O1
Mol. weight [g/mol]: 180.18
CAS: 51787-96-3

Physical Properties

Property code	Value	Unit	Source
gf	-230.87	kJ/mol	Joback Method
hf	-430.00	kJ/mol	Joback Method
hfus	19.81	kJ/mol	Joback Method
hvap	48.99	kJ/mol	Joback Method
log10ws	-2.66		Crippen Method
logp	2.204		Crippen Method
mcvol	126.350	ml/mol	McGowan Method
pc	3456.14	kPa	Joback Method
tb	569.18	K	Joback Method
tc	811.40	K	Joback Method
tf	347.68	K	Joback Method
vc	0.474	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.75	J/mol×K	569.18	Joback Method
cpg	323.26	J/mol×K	609.55	Joback Method
cpg	337.76	J/mol×K	649.92	Joback Method
cpg	351.25	J/mol×K	690.29	Joback Method
cpg	363.75	J/mol×K	730.66	Joback Method
cpg	375.27	J/mol×K	771.03	Joback Method
cpg	385.83	J/mol×K	811.40	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C51787963&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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