

«gamma»-tetradecalactone

Other names:	«gamma»-Tetradecanolide
Inchi:	InChI=1S/C14H26O2/c1-2-3-4-5-6-7-8-9-10-13-11-12-14(15)16-13/h13H,2-12H2,1H3
InchiKey:	AGNLJNRENXLLQO-UHFFFAOYSA-N
Formula:	C14H26O2
SMILES:	CCCCCCCCCCC1CCC(=O)O1
Mol. weight [g/mol]:	226.35

Physical Properties

Property code	Value	Unit	Source
gf	-105.16	kJ/mol	Joback Method
hf	-541.51	kJ/mol	Joback Method
hfus	33.44	kJ/mol	Joback Method
hvap	55.77	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	4.223		Crippen Method
mcvol	204.700	ml/mol	McGowan Method
pc	1801.56	kPa	Joback Method
rinpol	1920.00		NIST Webbook
rinpol	1912.00		NIST Webbook
rinpol	1877.00		NIST Webbook
rinpol	1920.00		NIST Webbook
rinpol	1912.00		NIST Webbook
ripol	2645.00		NIST Webbook
ripol	2645.00		NIST Webbook
ripol	2636.00		NIST Webbook
ripol	2628.00		NIST Webbook
ripol	2628.00		NIST Webbook
tb	629.77	K	Joback Method
tc	823.37	K	Joback Method
tf	353.23	K	Joback Method
vc	0.788	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	575.91	J/mol×K	629.77	Joback Method
cpg	595.32	J/mol×K	662.04	Joback Method
cpg	613.76	J/mol×K	694.30	Joback Method
cpg	631.25	J/mol×K	726.57	Joback Method
cpg	647.81	J/mol×K	758.84	Joback Method
cpg	663.46	J/mol×K	791.10	Joback Method
cpg	678.20	J/mol×K	823.37	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R210461&Units=SI

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

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