

5-Henicosyldihydrofuran-2(3H)-one

Inchi:	InChI=1S/C25H48O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-24-22-23
InchiKey:	FLVQHDPEFVLJND-UHFFFAOYSA-N
Formula:	C25H48O2
SMILES:	CCCCCCCCCCCCCCCCCCCC1CCC(=O)O1
Mol. weight [g/mol]:	380.65
CAS:	625835-46-3

Physical Properties

Property code	Value	Unit	Source
gf	-12.54	kJ/mol	Joback Method
hf	-768.55	kJ/mol	Joback Method
hfus	61.93	kJ/mol	Joback Method
hvap	80.26	kJ/mol	Joback Method
log10ws	-9.16		Crippen Method
logp	8.514		Crippen Method
mcvol	359.690	ml/mol	McGowan Method
pc	858.98	kPa	Joback Method
rinpol	3060.20		NIST Webbook
rinpol	3060.20		NIST Webbook
tb	881.45	K	Joback Method
tc	1079.67	K	Joback Method
tf	477.20	K	Joback Method
vc	1.405	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1238.34	J/mol×K	881.45	Joback Method
cpg	1260.40	J/mol×K	914.49	Joback Method
cpg	1281.04	J/mol×K	947.52	Joback Method
cpg	1300.32	J/mol×K	980.56	Joback Method
cpg	1318.28	J/mol×K	1013.60	Joback Method
cpg	1334.97	J/mol×K	1046.63	Joback Method
cpg	1350.42	J/mol×K	1079.67	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C625835463&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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