5-Docosyldihydrofuran-2(3H)-one

Inchi: InChI=1S/C26H50O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-25-23
InchiKey: KWOWNYUWWHKUCK-UHFFFAOYSA-N
Formula: C26H50O2
SMILES: CCCCCCCCCCCCCCCCCCCCCCCC1CCC(=O)O1
Mol. weight [g/mol]: 394.67
CAS: 52788-73-5

Physical Properties

Property code	Value	Unit	Source
gf	-4.12	kJ/mol	Joback Method
hf	-789.19	kJ/mol	Joback Method
hfus	64.52	kJ/mol	Joback Method
hvap	82.48	kJ/mol	Joback Method
log10ws	-9.57		Crippen Method
logp	8.904		Crippen Method
mcvol	373.780	ml/mol	McGowan Method
pc	812.61	kPa	Joback Method
rinpol	3157.70		NIST Webbook
rinpol	3157.70		NIST Webbook
tb	904.33	K	Joback Method
tc	1107.16	K	Joback Method
tf	488.47	K	Joback Method
vc	1.460	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1303.08	J/mol×K	904.33	Joback Method
cpg	1325.48	J/mol×K	938.13	Joback Method
cpg	1346.38	J/mol×K	971.94	Joback Method
cpg	1365.85	J/mol×K	1005.74	Joback Method
cpg	1383.92	J/mol×K	1039.55	Joback Method
cpg	1400.66	J/mol×K	1073.35	Joback Method
cpg	1416.10	J/mol×K	1107.16	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=C52788735&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume