6-heptyl-5,6-dihydro-2H-pyran-2-one

Inchi: InChI=1S/C12H20O2/c1-2-3-4-5-6-8-11-9-7-10-12(13)14-11/h7,10-11H,2-6,8-9H2,1H3
InchiKey: XPTXKXKPWKNYKB-UHFFFAOYSA-N
Formula: C12H20O2
SMILES: CCCCCCCC1CC=CC(=O)O1
Mol. weight [g/mol]: 196.29
CAS: 16400-72-9

Physical Properties

Property code	Value	Unit	Source
gf	-104.14	kJ/mol	Joback Method
hf	-448.61	kJ/mol	Joback Method
hfus	27.38	kJ/mol	Joback Method
hvap	51.78	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	3.219		Crippen Method
mcvol	172.220	ml/mol	McGowan Method
pc	2261.11	kPa	Joback Method
rinpol	1703.80		NIST Webbook
rinpol	1703.80		NIST Webbook
tb	587.44	K	Joback Method
tc	794.47	K	Joback Method
tf	327.93	K	Joback Method
vc	0.654	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	451.21	J/mol×K	587.44	Joback Method
cpg	469.61	J/mol×K	621.95	Joback Method
cpg	487.07	J/mol×K	656.45	Joback Method
cpg	503.60	J/mol×K	690.96	Joback Method
cpg	519.19	J/mol×K	725.46	Joback Method
cpg	533.86	J/mol×K	759.97	Joback Method
cpg	547.61	J/mol×K	794.47	Joback Method

Sources

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=C16400729&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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