6-Nonadecyltetrahydro-2H-pyran-2-one

Inchi: InChI=1S/C24H46O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-20-23-21-19-22-24
InchiKey: UKEXHCKUCRRCAR-UHFFFAOYSA-N
Formula: C24H46O2
SMILES: CCCCCCCCCCCCCCCCCCCC1CCCC(=O)O1
Mol. weight [g/mol]: 366.62
CAS: 159190-68-8

Physical Properties

Property code	Value	Unit	Source
gf	-33.06	kJ/mol	Joback Method
hf	-754.07	kJ/mol	Joback Method
hfus	57.24	kJ/mol	Joback Method
hvap	78.20	kJ/mol	Joback Method
log10ws	-8.74		Crippen Method
logp	8.124		Crippen Method
mcvol	345.600	ml/mol	McGowan Method
pc	923.30	kPa	Joback Method
rinpol	2999.50		NIST Webbook
rinpol	2999.50		NIST Webbook
tb	862.84	K	Joback Method
tc	1059.32	K	Joback Method
tf	462.41	K	Joback Method
vc	1.341	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1179.01	J/mol×K	862.84	Joback Method
cpg	1200.89	J/mol×K	895.59	Joback Method
cpg	1221.33	J/mol×K	928.33	Joback Method
cpg	1240.38	J/mol×K	961.08	Joback Method
cpg	1258.06	J/mol×K	993.83	Joback Method
cpg	1274.40	J/mol×K	1026.57	Joback Method
cpg	1289.45	J/mol×K	1059.32	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=C159190688&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