15-Nonacosanone

Other names: nonacosan-15-one
Inchi: InChI=1S/C29H58O/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29(30)28-26-24-22-20-18-1
InchiKey: FVKQALGTGOKSSK-UHFFFAOYSA-N
Formula: C29H58O
SMILES: CCCCCCCCCCCCCCC(=O)CCCCCCCCCCCCCC
Mol. weight [g/mol]: 422.77
CAS: 2764-73-0

Physical Properties

Property code	Value	Unit	Source
gf	64.38	kJ/mol	Joback Method
hf	-754.47	kJ/mol	Joback Method
hfus	72.47	kJ/mol	Joback Method
hvap	86.89	kJ/mol	Joback Method
log10ws	-11.24		Crippen Method
logp	10.738		Crippen Method
mcvol	421.040	ml/mol	McGowan Method
pc	644.51	kPa	Joback Method
rinpol	3096.90		NIST Webbook
tb	916.79	K	Joback Method
tc	1130.21	K	Joback Method
tf	466.52	K	Joback Method
vc	1.665	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1447.56	J/mol×K	916.79	Joback Method
cpg	1472.92	J/mol×K	952.36	Joback Method
cpg	1496.74	J/mol×K	987.93	Joback Method
cpg	1519.11	J/mol×K	1023.50	Joback Method
cpg	1540.12	J/mol×K	1059.07	Joback Method
cpg	1559.86	J/mol×K	1094.64	Joback Method
cpg	1578.41	J/mol×K	1130.21	Joback Method

dvisc	0.0008496	Pa×s	466.52	Joback Method
dvisc	0.0003200	Pa×s	541.56	Joback Method
dvisc	0.0001529	Pa×s	616.61	Joback Method
dvisc	0.0000857	Pa×s	691.65	Joback Method
dvisc	0.0000538	Pa×s	766.70	Joback Method
dvisc	0.0000367	Pa×s	841.75	Joback Method
dvisc	0.0000267	Pa×s	916.79	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=C2764730&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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