

Nonacosan-10-one

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

CAS:

InChI=1S/C29H58O/c1-3-5-7-9-11-12-13-14-15-16-17-18-19-20-22-24-26-28-29(30)27-2

ZPVRGRJHOPAZOE-UHFFFAOYSA-N

C29H58O

CCCCCCCCCCCCCCCCCCCC(=O)CCCCCCCCC

422.77

504-56-3

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	3089.90		NIST Webbook
rinpol	3089.90		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	1559.86	J/mol×K	1094.64	Joback Method
cpg	1540.12	J/mol×K	1059.07	Joback Method
cpg	1519.11	J/mol×K	1023.50	Joback Method
cpg	1496.74	J/mol×K	987.93	Joback Method
cpg	1472.92	J/mol×K	952.36	Joback Method
cpg	1578.41	J/mol×K	1130.21	Joback Method

dvisc	0.0000267	Pa×s	916.79	Joback Method
dvisc	0.0000367	Pa×s	841.75	Joback Method
dvisc	0.0000538	Pa×s	766.70	Joback Method
dvisc	0.0000857	Pa×s	691.65	Joback Method
dvisc	0.0001529	Pa×s	616.61	Joback Method
dvisc	0.0003200	Pa×s	541.56	Joback Method
dvisc	0.0008496	Pa×s	466.52	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C504563&Units=SI

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

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