

Nonacosan-14-one

Inchi:	InChI=1S/C29H58O/c1-3-5-7-9-11-13-15-16-18-20-22-24-26-28-29(30)27-25-23-21-19-1
InchiKey:	GHPAPAWCGDETKG-UHFFFAOYSA-N
Formula:	C29H58O
SMILES:	CCCCCCCCCCCCCCCC(=O)CCCCCCCCCCCC
Mol. weight [g/mol]:	422.77
CAS:	34394-11-1

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	3081.80		NIST Webbook
rinpol	3081.80		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/molxK	916.79	Joback Method
cpg	1472.92	J/molxK	952.36	Joback Method
cpg	1496.74	J/molxK	987.93	Joback Method
cpg	1519.11	J/molxK	1023.50	Joback Method
cpg	1540.12	J/molxK	1059.07	Joback Method
cpg	1559.86	J/molxK	1094.64	Joback Method
cpg	1578.41	J/molxK	1130.21	Joback Method

dvisc	0.0008496	Paxs	466.52	Joback Method
dvisc	0.0003200	Paxs	541.56	Joback Method
dvisc	0.0001529	Paxs	616.61	Joback Method
dvisc	0.0000857	Paxs	691.65	Joback Method
dvisc	0.0000538	Paxs	766.70	Joback Method
dvisc	0.0000367	Paxs	841.75	Joback Method
dvisc	0.0000267	Paxs	916.79	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=C34394111&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
mvol:	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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