

Octacosan-14-ol

Inchi:

InChI=1S/C28H58O/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-28(29)26-24-22-20-18-16-14

InchiKey:

JBKPMCOKLJUDQU-UHFFFAOYSA-N

Formula:

C28H58O

SMILES:

CCCCCCCCCCCCCCCC(O)CCCCCCCCCCCCCCC

Mol. weight [g/mol]:

410.76

CAS:

138967-02-9

Physical Properties

Property code	Value	Unit	Source
gf	45.62	kJ/mol	Joback Method
hf	-778.76	kJ/mol	Joback Method
hfus	68.84	kJ/mol	Joback Method
hvap	94.21	kJ/mol	Joback Method
log10ws	-10.92		Crippen Method
logp	10.140		Crippen Method
mcvol	411.250	ml/mol	McGowan Method
pc	690.34	kPa	Joback Method
rinpol	3010.30		NIST Webbook
tb	931.78	K	Joback Method
tc	1157.50	K	Joback Method
tf	451.14	K	Joback Method
vc	1.617	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1437.38	J/mol×K	931.78	Joback Method
cpg	1463.24	J/mol×K	969.40	Joback Method
cpg	1487.49	J/mol×K	1007.02	Joback Method
cpg	1510.24	J/mol×K	1044.64	Joback Method
cpg	1531.58	J/mol×K	1082.26	Joback Method
cpg	1551.63	J/mol×K	1119.88	Joback Method
cpg	1570.49	J/mol×K	1157.50	Joback Method
dvisc	0.0008767	Pa×s	451.14	Joback Method

dvisc	0.0001820	Pa×s	531.25	Joback Method
dvisc	0.0000570	Pa×s	611.35	Joback Method
dvisc	0.0000234	Pa×s	691.46	Joback Method
dvisc	0.0000115	Pa×s	771.57	Joback Method
dvisc	0.0000065	Pa×s	851.67	Joback Method
dvisc	0.0000040	Pa×s	931.78	Joback Method

Sources

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=C138967029&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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