1-Nonacosanol

Inchi: InChI=1S/C29H60O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-
InchiKey: PKBSGDQYUYBUDY-UHFFFAOYSA-N
Formula: C29H60O
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCO
Mol. weight [g/mol]: 424.79
CAS: 6624-76-6

Physical Properties

Property code	Value	Unit	Source
gf	56.48	kJ/mol	Joback Method
hf	-794.12	kJ/mol	Joback Method
hfus	74.95	kJ/mol	Joback Method
hvap	96.83	kJ/mol	Joback Method
log10ws	-11.23		Crippen Method
logp	10.531		Crippen Method
mcvol	425.340	ml/mol	McGowan Method
pc	654.10	kPa	Joback Method
tb	955.10	K	Joback Method
tc	1195.96	K	Joback Method
tf	357.75 ± 0.50	K	NIST Webbook
vc	1.679	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1503.56	J/mol×K	955.10	Joback Method
cpg	1531.01	J/mol×K	995.24	Joback Method
cpg	1556.66	J/mol×K	1035.39	Joback Method
cpg	1580.64	J/mol×K	1075.53	Joback Method
cpg	1603.09	J/mol×K	1115.67	Joback Method
cpg	1624.15	J/mol×K	1155.81	Joback Method
cpg	1643.94	J/mol×K	1195.96	Joback Method
dvisc	0.0005386	Pa×s	477.41	Joback Method
dvisc	0.0001295	Pa×s	557.02	Joback Method

dvisc	0.0000445	Pa×s	636.64	Joback Method
dvisc	0.0000194	Pa×s	716.25	Joback Method
dvisc	0.0000100	Pa×s	795.87	Joback Method
dvisc	0.0000058	Pa×s	875.49	Joback Method
dvisc	0.0000037	Pa×s	955.10	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53126e+01
Coeff. B	-6.41434e+03
Coeff. C	-1.44090e+02
Temperature range (K), min.	571.00
Temperature range (K), max.	785.45

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=C6624766&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume