Docosane, 9-octyl-

Other names: 9-Octyldocosane
9-n-Octyldocosane
Inchi: InChI=1S/C30H62/c1-4-7-10-13-16-17-18-19-20-23-26-29-30(27-24-21-14-11-8-5-2)28-2
InchiKey: RZCWYGUJADCQPF-UHFFFAOYSA-N
Formula: C30H62
SMILES: CCCCCCCCCCCCCC(CCCCCCCC)CCCCCCCC
Mol. weight [g/mol]: 422.81
CAS: 55319-83-0

Physical Properties

Property code	Value	Unit	Source
gf	199.28	kJ/mol	Joback Method
hf	-667.81	kJ/mol	Joback Method
hfus	69.93	kJ/mol	Joback Method
hvap	81.99	kJ/mol	Joback Method
log10ws	-12.14		Crippen Method
logp	11.805		Crippen Method
mcvol	433.560	ml/mol	McGowan Method
pc	597.80	kPa	Joback Method
tb	885.36	K	Joback Method
tc	1090.03	K	Joback Method
tf	281.80 ± 1.00	K	NIST Webbook
tf	281.80 ± 1.50	K	NIST Webbook
vc	1.710	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1623.76	J/mol×K	1090.03	Joback Method
cpg	1482.38	J/mol×K	885.36	Joback Method
cpg	1509.50	J/mol×K	919.47	Joback Method
cpg	1535.09	J/mol×K	953.58	Joback Method
cpg	1559.23	J/mol×K	987.69	Joback Method
cpg	1582.00	J/mol×K	1021.80	Joback Method

cpg	1603.48	J/mol×K	1055.92	Joback Method
dvisc	0.0000222	Pa×s	885.36	Joback Method
dvisc	0.0013422	Pa×s	412.86	Joback Method
dvisc	0.0003919	Pa×s	491.61	Joback Method
dvisc	0.0001607	Pa×s	570.36	Joback Method
dvisc	0.0000818	Pa×s	649.11	Joback Method
dvisc	0.0000482	Pa×s	727.86	Joback Method
dvisc	0.0000315	Pa×s	806.61	Joback Method
hvapt	109.30	kJ/mol	553.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.69944e+01
Coeff. B	-7.01535e+03
Coeff. C	-1.44090e+02
Temperature range (K), min.	564.00
Temperature range (K), max.	744.57

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C55319830&Units=SI

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

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

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
hvapt:	Enthalpy of vaporization at a given temperature
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