Hexadecane, 2-octyl

Other names: 9-methyltricosane
Inchi: InChI=1S/C24H50/c1-4-6-8-10-12-13-14-15-16-17-19-21-23-24(3)22-20-18-11-9-7-5-2/h2
InchiKey: LONYBAXSVHLIBH-UHFFFAOYSA-N
Formula: C24H50
SMILES: CCCCCCCCCCCCCCC(C)CCCCCCCC
Mol. weight [g/mol]: 338.65

Physical Properties

Property code	Value	Unit	Source
gf	148.76	kJ/mol	Joback Method
hf	-543.97	kJ/mol	Joback Method
hfus	54.39	kJ/mol	Joback Method
hvap	68.63	kJ/mol	Joback Method
log10ws	-9.63		Crippen Method
logp	9.464		Crippen Method
mcvol	349.020	ml/mol	McGowan Method
pc	809.83	kPa	Joback Method
rinpol	2335.00		NIST Webbook
rinpol	2337.00		NIST Webbook
rinpol	2337.00		NIST Webbook
tb	748.08	K	Joback Method
tc	918.22	K	Joback Method
tf	345.24	K	Joback Method
vc	1.373	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1087.86	J/mol×K	748.08	Joback Method
cpg	1110.78	J/mol×K	776.44	Joback Method
cpg	1132.66	J/mol×K	804.79	Joback Method
cpg	1153.54	J/mol×K	833.15	Joback Method
cpg	1173.45	J/mol×K	861.51	Joback Method
cpg	1192.43	J/mol×K	889.86	Joback Method

cpg	1210.52	J/mol×K	918.22	Joback Method
dvisc	0.0031119	Pa×s	345.24	Joback Method
dvisc	0.0009096	Pa×s	412.38	Joback Method
dvisc	0.0003752	Pa×s	479.52	Joback Method
dvisc	0.0001924	Pa×s	546.66	Joback Method
dvisc	0.0001142	Pa×s	613.80	Joback Method
dvisc	0.0000751	Pa×s	680.94	Joback Method
dvisc	0.0000532	Pa×s	748.08	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=R47568&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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