

12-heptyltricosane

Inchi:

InChI=1S/C30H62/c1-4-7-10-13-15-17-19-22-25-28-30(27-24-21-12-9-6-3)29-26-23-20-1

InchiKey:

CWEMFZROPOWTNA-UHFFFAOYSA-N

Formula:

C30H62

SMILES:

CCCCCCCCCCCC(CCCCCC)CCCCCCCCCCCC

Mol. weight [g/mol]:

422.81

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
rinpol	2839.00		NIST Webbook
tb	885.36	K	Joback Method
tc	1090.03	K	Joback Method
tf	412.86	K	Joback Method
vc	1.710	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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
cpg	1623.76	J/mol×K	1090.03	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
dvisc	0.0000222	Pa×s	885.36	Joback Method

Sources

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=R248203&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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