

3,7,11,15-tetramethyl-nonacosane

Inchi:

InChI=1S/C33H68/c1-7-9-10-11-12-13-14-15-16-17-18-19-23-31(4)26-21-27-33(6)29-22-

InchiKey:

GGBBYBPFYIFTSD-UHFFFAOYSA-N

Formula:

C33H68

SMILES:

CCCCCCCCCCCCCCCC(C)CCCC(C)CCCC(C)CCCC(C)CC

Mol. weight [g/mol]:

464.89

Physical Properties

Property code	Value	Unit	Source
gf	217.22	kJ/mol	Joback Method
hf	-745.57	kJ/mol	Joback Method
hfus	67.13	kJ/mol	Joback Method
hvap	87.50	kJ/mol	Joback Method
log10ws	-12.67		Crippen Method
logp	12.543		Crippen Method
mcvol	475.830	ml/mol	McGowan Method
pc	527.50	kPa	Joback Method
rinpol	3060.00		NIST Webbook
rinpol	3062.00		NIST Webbook
rinpol	3060.00		NIST Webbook
rinpol	3062.00		NIST Webbook
rinpol	3062.00		NIST Webbook
tb	952.68	K	Joback Method
tc	1181.52	K	Joback Method
tf	401.67	K	Joback Method
vc	1.859	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1687.83	J/mol×K	952.68	Joback Method
cpg	1717.20	J/mol×K	990.82	Joback Method
cpg	1744.67	J/mol×K	1028.96	Joback Method
cpg	1770.35	J/mol×K	1067.10	Joback Method
cpg	1794.37	J/mol×K	1105.24	Joback Method

cpg	1816.87	J/mol×K	1143.38	Joback Method
cpg	1837.96	J/mol×K	1181.52	Joback Method
dvisc	0.0018040	Pa×s	401.67	Joback Method
dvisc	0.0003453	Pa×s	493.50	Joback Method
dvisc	0.0001110	Pa×s	585.34	Joback Method
dvisc	0.0000486	Pa×s	677.17	Joback Method
dvisc	0.0000259	Pa×s	769.01	Joback Method
dvisc	0.0000158	Pa×s	860.85	Joback Method
dvisc	0.0000106	Pa×s	952.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R300331&Units=SI
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

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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