

Pentyl triacontyl ether

Inchi:

InChI=1S/C35H72O/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-26

InchiKey:

JOJLNMKWLXUOAL-UHFFFAOYSA-N

Formula:

C35H72O

SMILES:

CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCOCCCCC

Mol. weight [g/mol]:

508.95

Physical Properties

Property code	Value	Unit	Source
gf	138.82	kJ/mol	Joback Method
hf	-897.95	kJ/mol	Joback Method
hfus	87.59	kJ/mol	Joback Method
hvap	95.91	kJ/mol	Joback Method
log10ws	-13.56		Crippen Method
logp	13.136		Crippen Method
mcvol	509.880	ml/mol	McGowan Method
pc	473.62	kPa	Joback Method
rinpol	3765.00		NIST Webbook
rinpol	3765.00		NIST Webbook
tb	1022.62	K	Joback Method
tc	1307.47	K	Joback Method
tf	506.44	K	Joback Method
vc	2.014	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1860.76	J/mol×K	1022.62	Joback Method
cpg	2003.63	J/mol×K	1260.00	Joback Method
cpg	1979.96	J/mol×K	1212.52	Joback Method
cpg	1954.07	J/mol×K	1165.05	Joback Method
cpg	1925.72	J/mol×K	1117.57	Joback Method
cpg	1894.69	J/mol×K	1070.10	Joback Method
cpg	2025.29	J/mol×K	1307.47	Joback Method
dvisc	0.0000082	Pa×s	1022.62	Joback Method

dvisc	0.0000114	Pa×s	936.59	Joback Method
dvisc	0.0000171	Pa×s	850.56	Joback Method
dvisc	0.0000280	Pa×s	764.53	Joback Method
dvisc	0.0000519	Pa×s	678.50	Joback Method
dvisc	0.0001153	Pa×s	592.47	Joback Method
dvisc	0.0003357	Pa×s	506.44	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406425&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
mccvol:	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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