Pentatricosane, 17-methyl

Inchi: InChI=1S/C36H74/c1-4-6-8-10-12-14-16-18-20-21-23-25-27-29-31-33-35-36(3)34-32-30-
InchiKey: QLUGCBLRPGWWHD-UHFFFAOYSA-N
Formula: C36H74
SMILES: CCCCCCCCCCCCCCCCCCC(C)CCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 506.97

Physical Properties

Property code	Value	Unit	Source
gf	249.80	kJ/mol	Joback Method
hf	-791.65	kJ/mol	Joback Method
hfus	85.47	kJ/mol	Joback Method
hvap	95.34	kJ/mol	Joback Method
log10ws	-14.65		Crippen Method
logp	14.146		Crippen Method
mcvol	518.100	ml/mol	McGowan Method
pc	459.31	kPa	Joback Method
rinpol	3531.00		NIST Webbook
rinpol	3531.00		NIST Webbook
tb	1022.64	K	Joback Method
tc	1304.31	K	Joback Method
tf	480.48	K	Joback Method
vc	2.046	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1895.00	J/mol×K	1022.64	Joback Method
cpg	1929.92	J/mol×K	1069.59	Joback Method
cpg	1962.18	J/mol×K	1116.53	Joback Method
cpg	1992.06	J/mol×K	1163.48	Joback Method
cpg	2019.81	J/mol×K	1210.42	Joback Method
cpg	2045.68	J/mol×K	1257.37	Joback Method
cpg	2069.95	J/mol×K	1304.31	Joback Method
dvisc	0.0005358	Pa×s	480.48	Joback Method

dvisc	0.0001564	Pa×s	570.84	Joback Method
dvisc	0.0000639	Pa×s	661.20	Joback Method
dvisc	0.0000324	Pa×s	751.56	Joback Method
dvisc	0.0000190	Pa×s	841.92	Joback Method
dvisc	0.0000123	Pa×s	932.28	Joback Method
dvisc	0.0000087	Pa×s	1022.64	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=R609019&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