5-methyltritriacontane

Other names: 5-Methyltritriacontane
Inchi: InChI=1S/C34H70/c1-4-6-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-26-27-
InchiKey: FPKNBTAWMQVIIW-UHFFFAOYSA-N
Formula: C34H70
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCCC(C)CCCC
Mol. weight [g/mol]: 478.92
CAS: 500024-69-1

Physical Properties

Property code	Value	Unit	Source
af	1.3080		Cheméo Relay (1.0)
gf	232.96	kJ/mol	Joback Method
hf	-757.26	kJ/mol	Cheméo Relay (1.0)
hfus	80.29	kJ/mol	Joback Method
hvap	165.18	kJ/mol	Cheméo Relay (1.0)
ie	10.23	eV	Cheméo Relay (1.0)
log10ws	-12.38		Cheméo Relay (1.0)
logp	13.365		Crippen Method
mcvol	489.920	ml/mol	McGowan Method
pc	499.58	kPa	Joback Method
tb	663.45	K	Cheméo Relay (1.0)
tc	833.50	K	Cheméo Relay (1.0)
tf	328.80 ± 0.50	K	NIST Webbook
vc	1.929	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1756.03	J/mol×K	976.88	Joback Method
cpg	1787.83	J/mol×K	1018.53	Joback Method
cpg	1817.45	J/mol×K	1060.18	Joback Method
cpg	1845.07	J/mol×K	1101.83	Joback Method
cpg	1870.84	J/mol×K	1143.48	Joback Method
cpg	1894.95	J/mol×K	1185.12	Joback Method

cpg	1917.55	J/mol×K	1226.77	Joback Method
dvisc	0.0007325	Pa×s	457.94	Joback Method
dvisc	0.0002138	Pa×s	544.43	Joback Method
dvisc	0.0000875	Pa×s	630.92	Joback Method
dvisc	0.0000444	Pa×s	717.41	Joback Method
dvisc	0.0000261	Pa×s	803.90	Joback Method
dvisc	0.0000170	Pa×s	890.39	Joback Method
dvisc	0.0000119	Pa×s	976.88	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C500024691&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume