16-Nonatricosene, 27-methyl

Inchi: InChI=1S/C40H80/c1-4-6-8-10-12-14-16-17-18-19-20-21-22-23-24-25-26-27-28-29-31-33
InchiKey: ZCANRQAGEKVESN-OCOZRVBESA-N
Formula: C40H80
SMILES: CCCCCCCCCCCCCCCC=CCCCCCCCCCC(C)CCCCCCCCCCC
Mol. weight [g/mol]: 561.06

Physical Properties

Property code	Value	Unit	Source
gf	363.70	kJ/mol	Joback Method
hf	-756.99	kJ/mol	Joback Method
hfus	96.04	kJ/mol	Joback Method
hvap	104.20	kJ/mol	Joback Method
log10ws	-16.18		Crippen Method
logp	15.482		Crippen Method
mcvol	570.160	ml/mol	McGowan Method
pc	400.32	kPa	Joback Method
rinpol	3902.00		NIST Webbook
tb	1118.32	K	Joback Method
tc	1477.35	K	Joback Method
tf	520.48	K	Joback Method
vc	2.249	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2148.80	J/mol×K	1118.32	Joback Method
cpg	2191.40	J/mol×K	1178.16	Joback Method
cpg	2230.91	J/mol×K	1238.00	Joback Method
cpg	2268.00	J/mol×K	1297.83	Joback Method
cpg	2303.33	J/mol×K	1357.67	Joback Method
cpg	2337.54	J/mol×K	1417.51	Joback Method
cpg	2371.30	J/mol×K	1477.35	Joback Method
dvisc	0.0002659	Pa×s	520.48	Joback Method
dvisc	0.0000752	Pa×s	620.12	Joback Method

dvisc	0.0000302	Pa×s	719.76	Joback Method
dvisc	0.0000151	Pa×s	819.40	Joback Method
dvisc	0.0000088	Pa×s	919.04	Joback Method
dvisc	0.0000057	Pa×s	1018.68	Joback Method
dvisc	0.0000040	Pa×s	1118.32	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R608561&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