Heneicosane, 2-methyl

Inchi: InChI=1S/C22H46/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22(2)3/h22H,4-
InchiKey: JQMPJOXNMWUULP-UHFFFAOYSA-N
Formula: C22H46
SMILES: CCCCCCCCCCCCCCCCCCCC(C)C
Mol. weight [g/mol]: 310.60

Physical Properties

Property code	Value	Unit	Source
gf	131.92	kJ/mol	Joback Method
hf	-502.69	kJ/mol	Joback Method
hfus	49.21	kJ/mol	Joback Method
hvap	64.18	kJ/mol	Joback Method
log10ws	-8.79		Crippen Method
logp	8.684		Crippen Method
mcvol	320.840	ml/mol	McGowan Method
pc	906.15	kPa	Joback Method
rinpol	2160.00		NIST Webbook
rinpol	2166.00		NIST Webbook
rinpol	2165.20		NIST Webbook
rinpol	2163.00		NIST Webbook
rinpol	2166.00		NIST Webbook
rinpol	2162.00		NIST Webbook
rinpol	2166.00		NIST Webbook
rinpol	2165.20		NIST Webbook
rinpol	2164.00		NIST Webbook
tb	702.32	K	Joback Method
tc	867.26	K	Joback Method
tf	322.70	K	Joback Method
vc	1.262	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	962.39	J/mol×K	702.32	Joback Method

cpg	984.38	J/mol×K	729.81	Joback Method
cpg	1005.42	J/mol×K	757.30	Joback Method
cpg	1025.55	J/mol×K	784.79	Joback Method
cpg	1044.78	J/mol×K	812.28	Joback Method
cpg	1063.16	J/mol×K	839.77	Joback Method
cpg	1080.72	J/mol×K	867.26	Joback Method
dvisc	0.0040182	Pa×s	322.70	Joback Method
dvisc	0.0011754	Pa×s	385.97	Joback Method
dvisc	0.0004861	Pa×s	449.24	Joback Method
dvisc	0.0002500	Pa×s	512.51	Joback Method
dvisc	0.0001488	Pa×s	575.78	Joback Method
dvisc	0.0000982	Pa×s	639.05	Joback Method
dvisc	0.0000698	Pa×s	702.32	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=R47433&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