4-Methyleicosane

Inchi: InChI=1S/C21H44/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-18-20-21(3)19-5-2/h21H,4-20H
InchiKey: XLKVRUORNFWTNM-UHFFFAOYSA-N
Formula: C21H44
SMILES: CCCCCCCCCCCCCCCCC(C)CCC
Mol. weight [g/mol]: 296.57
CAS: 25117-28-6

Physical Properties

Property code	Value	Unit	Source
af	0.8502		Cheméo Relay (1.0)
gf	123.50	kJ/mol	Joback Method
hf	-484.72	kJ/mol	Cheméo Relay (1.0)
hfus	46.62	kJ/mol	Joback Method
hvap	101.62	kJ/mol	Cheméo Relay (1.0)
ie	9.79	eV	Cheméo Relay (1.0)
log10ws	-8.84		Cheméo Relay (1.0)
logp	8.294		Crippen Method
mcvol	306.750	ml/mol	McGowan Method
pc	960.88	kPa	Joback Method
tb	581.54	K	Cheméo Relay (1.0)
tc	752.08	K	Cheméo Relay (1.0)
tf	278.32	K	Cheméo Relay (1.0)
vc	1.209	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	901.08	J/mol×K	679.44	Joback Method
cpg	922.65	J/mol×K	706.64	Joback Method
cpg	943.32	J/mol×K	733.85	Joback Method
cpg	963.10	J/mol×K	761.05	Joback Method
cpg	982.02	J/mol×K	788.26	Joback Method
cpg	1000.12	J/mol×K	815.46	Joback Method
cpg	1017.42	J/mol×K	842.66	Joback Method

dvisc	0.0045387	Pa×s	311.43	Joback Method
dvisc	0.0013283	Pa×s	372.76	Joback Method
dvisc	0.0005501	Pa×s	434.10	Joback Method
dvisc	0.0002834	Pa×s	495.44	Joback Method
dvisc	0.0001690	Pa×s	556.77	Joback Method
dvisc	0.0001116	Pa×s	618.11	Joback Method
dvisc	0.0000795	Pa×s	679.44	Joback Method
hvapt	70.20	kJ/mol	546.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.83383e+01
Coeff. B	-8.56957e+03
Coeff. C	3.40300e+00
Temperature range (K), min.	471.35
Temperature range (K), max.	654.44

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C25117286&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
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):

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
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume