Eicosane, 3-methyl-

Other names: 3-Methyleicosane
Inchi: InChI=1S/C21H44/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21(3)5-2/h21H,4-20H
InchiKey: GZCXIMGMPAZPPM-UHFFFAOYSA-N
Formula: C21H44
SMILES: CCCCCCCCCCCCCCCCCC(C)CC
Mol. weight [g/mol]: 296.57
CAS: 6418-46-8

Physical Properties

Property code	Value	Unit	Source
gf	123.50	kJ/mol	Joback Method
hf	-482.05	kJ/mol	Joback Method
hfus	46.62	kJ/mol	Joback Method
hvap	61.95	kJ/mol	Joback Method
log10ws	-8.37		Crippen Method
logp	8.294		Crippen Method
mcvol	306.750	ml/mol	McGowan Method
pc	960.88	kPa	Joback Method
rinpol	2072.00		NIST Webbook
rinpol	2072.00		NIST Webbook
rinpol	2062.00		NIST Webbook
rinpol	2068.00		NIST Webbook
rinpol	2074.00		NIST Webbook
rinpol	2069.00		NIST Webbook
rinpol	2068.00		NIST Webbook
rinpol	2068.00		NIST Webbook
rinpol	2074.20		NIST Webbook
rinpol	2065.00		NIST Webbook
rinpol	2074.00		NIST Webbook
tb	679.44	K	Joback Method
tc	842.66	K	Joback Method
tf	286.45	K	NIST Webbook
tf	286.50 ± 0.50	K	NIST Webbook
vc	1.206	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1017.42	J/mol×K	842.66	Joback Method
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
dvisc	0.0000795	Pa×s	679.44	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
hvapt	74.50	kJ/mol	548.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.91820e+01
Coeff. B	-9.03580e+03
Coeff. C	1.84000e-01
Temperature range (K), min.	478.04
Temperature range (K), max.	651.25

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6418468&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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

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