CYCLOEICOSANE

Inchi: InChI=1S/C20H40/c1-2-4-6-8-10-12-14-16-18-20-19-17-15-13-11-9-7-5-3-1/h1-20H2
InchiKey: ZBLGFUHEYYJSSE-UHFFFAOYSA-N
Formula: C20H40
SMILES: C1CCCCCCCCCCCCCCCCCCCC1
Mol. weight [g/mol]: 280.54
CAS: 296-56-0

Physical Properties

Property code	Value	Unit	Source
af	0.2321		Cheméo Relay (1.0)
gf	-19.72	kJ/mol	Joback Method
hf	-468.53	kJ/mol	Cheméo Relay (1.0)
hfus	8.92	kJ/mol	Joback Method
hvap	85.86	kJ/mol	Cheméo Relay (1.0)
ie	9.58	eV	Cheméo Relay (1.0)
log10ws	-7.46		Cheméo Relay (1.0)
logp	7.802		Crippen Method
mcvol	281.800	ml/mol	McGowan Method
pc	1537.87	kPa	Joback Method
tb	667.20	K	Cheméo Relay (1.0)
tc	835.27	K	Cheméo Relay (1.0)
tf	335.00 ± 3.00	K	NIST Webbook
vc	0.935	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	897.51	J/mol×K	741.00	Joback Method
cpg	933.12	J/mol×K	785.07	Joback Method
cpg	965.18	J/mol×K	829.14	Joback Method
cpg	993.62	J/mol×K	873.21	Joback Method
cpg	1018.35	J/mol×K	917.28	Joback Method
cpg	1039.29	J/mol×K	961.36	Joback Method
cpg	1056.36	J/mol×K	1005.43	Joback Method

dvisc	0.2197498	Pa×s	277.50	Joback Method
dvisc	0.0028155	Pa×s	354.75	Joback Method
dvisc	0.0001714	Pa×s	432.00	Joback Method
dvisc	0.0000244	Pa×s	509.25	Joback Method
dvisc	0.0000058	Pa×s	586.50	Joback Method
dvisc	0.0000019	Pa×s	663.75	Joback Method
dvisc	0.0000008	Pa×s	741.00	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.28415e+01
Coeff. B	-4.36751e+03
Coeff. C	-1.00270e+02
Temperature range (K), min.	448.17
Temperature range (K), max.	680.28

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C296560&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):

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

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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume