

1-Eicosene

Other names:	1-Icosene CETYLETHYLENE Cetyl ethylene EICOSENE Eicos-1-ene Icos-1-ene NSC 77138 Neodene 20 «alpha»-Eicosene Â«alphaÂ»-Eicosene
Inchi:	InChI=1S/C20H40/c1-3-5-7-9-11-13-15-17-19-20-18-16-14-12-10-8-6-4-2/h3H,1,4-20H2,
InchiKey:	VAMFXQBUQXONLZ-UHFFFAOYSA-N
Formula:	C20H40
SMILES:	C=CCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	280.53
CAS:	3452-07-1

Physical Properties

Property code	Value	Unit	Source
af	0.7700		KDB
gf	205.36	kJ/mol	Joback Method
hf	-330.70	kJ/mol	Joback Method
hfus	46.28	kJ/mol	Joback Method
hvap	100.00	kJ/mol	NIST Webbook
log10ws	-8.05		Crippen Method
logp	7.824		Crippen Method
mcvol	288.360	ml/mol	McGowan Method
pc	1040.00	kPa	KDB
rinpol	1993.00		NIST Webbook
rinpol	1992.00		NIST Webbook
rinpol	1994.00		NIST Webbook
rinpol	1994.00		NIST Webbook
rinpol	1989.00		NIST Webbook
rinpol	1994.00		NIST Webbook
rinpol	1988.00		NIST Webbook
rinpol	1993.00		NIST Webbook
rinpol	1996.00		NIST Webbook

rinpol	1988.00		NIST Webbook
rinpol	1997.00		NIST Webbook
rinpol	1991.00		NIST Webbook
rinpol	1989.00		NIST Webbook
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rinpol	1994.00		NIST Webbook
rinpol	1986.00		NIST Webbook
rinpol	1996.00		NIST Webbook
rinpol	1992.00		NIST Webbook
rinpol	1994.00		NIST Webbook
rinpol	1987.00		NIST Webbook
rinpol	1994.00		NIST Webbook
rinpol	1988.00		NIST Webbook
rinpol	2000.00		NIST Webbook
rinpol	1991.00		NIST Webbook
rinpol	2000.00		NIST Webbook
rinpol	1988.00		NIST Webbook
rinpol	1995.00		NIST Webbook
rinpol	1997.00		NIST Webbook
ripol	2047.00		NIST Webbook
ripol	2056.00		NIST Webbook
ripol	2058.00		NIST Webbook
ripol	2047.00		NIST Webbook
tb	614.20	K	NIST Webbook
tb	614.90	K	KDB
tc	765.40	K	KDB
tf	302.00	K	KDB
vc	1.165	m3/kmol	KDB
zc	0.1903040		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	816.83	J/mol×K	653.68	Joback Method
cpg	837.29	J/mol×K	680.63	Joback Method

cpg	856.90	J/mol×K	707.58	Joback Method
cpg	875.68	J/mol×K	734.52	Joback Method
cpg	893.67	J/mol×K	761.47	Joback Method
cpg	910.89	J/mol×K	788.42	Joback Method
cpg	927.37	J/mol×K	815.37	Joback Method
dvisc	0.0012341	Pa×s	370.11	Joback Method
dvisc	0.0034940	Pa×s	313.40	Joback Method
dvisc	0.0005748	Pa×s	426.83	Joback Method
dvisc	0.0003202	Pa×s	483.54	Joback Method
dvisc	0.0002017	Pa×s	540.25	Joback Method
dvisc	0.0001388	Pa×s	596.97	Joback Method
dvisc	0.0001018	Pa×s	653.68	Joback Method
hvapt	56.07	kJ/mol	614.90	KDB
hvapt	74.30	kJ/mol	558.00	NIST Webbook
hvapt	65.00	kJ/mol	594.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	424.20	K	0.10	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.52499e+01
Coeff. B	-5.33020e+03
Coeff. C	-1.12846e+02
Temperature range (K), min.	469.09
Temperature range (K), max.	649.17

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C*\ln(T) + D*T^2$
Coeff. A	2.30379e+02
Coeff. B	-2.13481e+04

Coeff. C	-3.03848e+01
Coeff. D	1.07740e-05
Temperature range (K), min.	301.76
Temperature range (K), max.	771.00

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=355
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemed.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.thermo.com/files/research/kdb/mol/mol355.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3452071&Units=SI

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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

zc: Critical Compressibility

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