

3-Eicosyne

Inchi:

InChI=1S/C20H38/c1-3-5-7-9-11-13-15-17-19-20-18-16-14-12-10-8-6-4-2/h3-5,7,9-20H2

InchiKey:

AQBXRWJMJJJCLI-UHFFFAOYSA-N

Formula:

C20H38

SMILES:

CCC#CCCCCCCCCCCCCCCCC

Mol. weight [g/mol]:

278.52

CAS:

61886-66-6

Physical Properties

Property code	Value	Unit	Source
gf	320.32	kJ/mol	Joback Method
hf	-183.83	kJ/mol	Joback Method
hfus	50.68	kJ/mol	Joback Method
hvap	62.27	kJ/mol	Joback Method
log10ws	-7.99		Crippen Method
logp	7.271		Crippen Method
mcvol	284.060	ml/mol	McGowan Method
pc	1127.59	kPa	Joback Method
rinpol	1987.00		NIST Webbook
rinpol	1989.00		NIST Webbook
tb	666.00	K	Joback Method
tc	837.81	K	Joback Method
tf	421.26	K	Joback Method
vc	1.117	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	800.08	J/mol×K	666.00	Joback Method
cpg	820.62	J/mol×K	694.63	Joback Method
cpg	840.26	J/mol×K	723.27	Joback Method
cpg	859.05	J/mol×K	751.90	Joback Method
cpg	877.00	J/mol×K	780.54	Joback Method
cpg	894.15	J/mol×K	809.17	Joback Method
cpg	910.52	J/mol×K	837.81	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.46986e+01
Coeff. B	-5.09710e+03
Coeff. C	-1.08826e+02
Temperature range (K), min.	462.52
Temperature range (K), max.	651.81

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6188666&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
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
mccvol:	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

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