

1-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/h1H,4-20H2,2H
InchiKey:	BUSHLWVWPAEVMX-UHFFFAOYSA-N
Formula:	C20H38
SMILES:	C#CCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	278.52
CAS:	765-27-5

Physical Properties

Property code	Value	Unit	Source
af	0.7500		KDB
gf	340.59	kJ/mol	Joback Method
hf	-164.23	kJ/mol	Joback Method
hfus	50.53	kJ/mol	Joback Method
hvap	59.97	kJ/mol	Joback Method
log10ws	-7.99		Crippen Method
logp	7.271		Crippen Method
mcvol	284.060	ml/mol	McGowan Method
pc	1120.00	kPa	KDB
tb	613.20	K	KDB
tb	587.65 ± 3.00	K	NIST Webbook
tc	769.80	K	KDB
tf	309.00	K	KDB
vc	1.117	m ³ /kmol	KDB
zc	0.1955470		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	792.22	J/mol×K	647.12	Joback Method
cpg	812.33	J/mol×K	674.67	Joback Method
cpg	831.59	J/mol×K	702.22	Joback Method
cpg	850.02	J/mol×K	729.77	Joback Method
cpg	867.66	J/mol×K	757.32	Joback Method
cpg	884.53	J/mol×K	784.87	Joback Method

cpg	900.67	J/mol×K	812.43	Joback Method
hvapt	68.90	kJ/mol	562.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.54166e+01
Coeff. B	-5.43009e+03
Coeff. C	-1.11608e+02
Temperature range (K), min.	470.53
Temperature range (K), max.	648.97

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.thermo.com/files/research/kdb/mol/mol445.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C765275&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/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af:	Acentric Factor
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

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
zc:	Critical Compressibility

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