

3-Eicosanone

Inchi:	InChI=1S/C20H40O/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20(21)4-2/h3-19H2,
InchiKey:	BWVLRRQCABCGBO-UHFFFAOYSA-N
Formula:	C20H40O
SMILES:	CCCCCCCCCCCCCCCC(=O)CC
Mol. weight [g/mol]:	296.53
CAS:	2955-56-8

Physical Properties

Property code	Value	Unit	Source
gf	-11.40	kJ/mol	Joback Method
hf	-568.71	kJ/mol	Joback Method
hfus	49.16	kJ/mol	Joback Method
hvap	66.86	kJ/mol	Joback Method
log10ws	-7.47		Crippen Method
logp	7.227		Crippen Method
mcvol	294.230	ml/mol	McGowan Method
pc	1057.57	kPa	Joback Method
tb	710.87	K	Joback Method
tc	880.03	K	Joback Method
tf	334.15 ± 1.50	K	NIST Webbook
vc	1.161	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	875.44	J/mol×K	710.87	Joback Method
cpg	895.27	J/mol×K	739.06	Joback Method
cpg	914.21	J/mol×K	767.26	Joback Method
cpg	932.27	J/mol×K	795.45	Joback Method
cpg	949.51	J/mol×K	823.64	Joback Method
cpg	965.93	J/mol×K	851.83	Joback Method
cpg	981.58	J/mol×K	880.03	Joback Method
dvisc	0.0024837	Paxs	365.09	Joback Method
dvisc	0.0009987	Paxs	422.72	Joback Method

dvisc	0.0004997	Paxs	480.35	Joback Method
dvisc	0.0002900	Paxs	537.98	Joback Method
dvisc	0.0001870	Paxs	595.61	Joback Method
dvisc	0.0001303	Paxs	653.24	Joback Method
dvisc	0.0000962	Paxs	710.87	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.44932e+01
Coeff. B	-5.15102e+03
Coeff. C	-1.14636e+02
Temperature range (K), min.	477.24
Temperature range (K), max.	675.64

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2955568&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
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

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