2-Eicosanone

Inchi: InChI=1S/C20H40O/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20(2)21/h3-19H2,1
InchiKey: GARHHHWGJIXLDK-UHFFFAOYSA-N
Formula: C20H40O
SMILES: CCCCCCCCCCCCCCCCCCC(C)=O
Mol. weight [g/mol]: 296.53
CAS: 29703-52-4

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
rinpol	2206.00		NIST Webbook
rinpol	362.51		NIST Webbook
rinpol	2206.00		NIST Webbook
tb	710.87	K	Joback Method
tc	880.03	K	Joback Method
tf	365.09	K	Joback Method
vc	1.161	m3/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	Pa×s	365.09	Joback Method
dvisc	0.0009987	Pa×s	422.72	Joback Method
dvisc	0.0004997	Pa×s	480.35	Joback Method
dvisc	0.0002900	Pa×s	537.98	Joback Method
dvisc	0.0001870	Pa×s	595.61	Joback Method
dvisc	0.0001303	Pa×s	653.24	Joback Method
dvisc	0.0000962	Pa×s	710.87	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47541e+01
Coeff. B	-5.27580e+03
Coeff. C	-1.15748e+02
Temperature range (K), min.	480.44
Temperature range (K), max.	674.47

Sources

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C29703524&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume