

2-Heneicosanone

Inchi:	InChI=1S/C21H42O/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21(2)22/h3-20H
InchiKey:	VUVUIDMZOWHIIJ-UHFFFAOYSA-N
Formula:	C21H42O
SMILES:	CCCCCCCCCCCCCCCCCCC(C)=O
Mol. weight [g/mol]:	310.56
CAS:	---

Physical Properties

Property code	Value	Unit	Source
gf	-2.98	kJ/mol	Joback Method
hf	-589.35	kJ/mol	Joback Method
hfus	51.74	kJ/mol	Joback Method
hvap	69.09	kJ/mol	Joback Method
log10ws	-7.89		Crippen Method
logp	7.617		Crippen Method
mcvol	308.320	ml/mol	McGowan Method
pc	994.51	kPa	Joback Method
rinpol	376.32		NIST Webbook
rinpol	2309.00		NIST Webbook
rinpol	2309.00		NIST Webbook
tb	733.75	K	Joback Method
tc	904.73	K	Joback Method
tf	376.36	K	Joback Method
vc	1.218	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	935.81	J/mol×K	733.75	Joback Method
cpg	956.07	J/mol×K	762.25	Joback Method
cpg	975.40	J/mol×K	790.74	Joback Method
cpg	993.82	J/mol×K	819.24	Joback Method
cpg	1011.38	J/mol×K	847.74	Joback Method
cpg	1028.09	J/mol×K	876.23	Joback Method

cpg	1044.00	J/mol×K	904.73	Joback Method
dvisc	0.0022413	Pa×s	376.36	Joback Method
dvisc	0.0008932	Pa×s	435.93	Joback Method
dvisc	0.0004441	Pa×s	495.49	Joback Method
dvisc	0.0002565	Pa×s	555.06	Joback Method
dvisc	0.0001648	Pa×s	614.62	Joback Method
dvisc	0.0001145	Pa×s	674.18	Joback Method
dvisc	0.0000844	Pa×s	733.75	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.46438e+01
Coeff. B	-5.31504e+03
Coeff. C	-1.18695e+02
Temperature range (K), min.	488.92
Temperature range (K), max.	688.22

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R84897&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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