11-Heneicosanone

Other names:	di-n-Decyl ketone
	Didecyl ketone
	henicosan-11-one
Inchi:	InChI=1S/C21H42O/c1-3-5-7-9-11-13-15-17-19-21(22)20-18-16-14-12-10-8-6-4-2/h3-20H
InchiKey:	DOACSXJVHDTDSG-UHFFFAOYSA-N
Formula:	C21H42O
SMILES:	CCCCCCCCCCC(=O)CCCCCCCCCC
Mol. weight [g/mol]:	310.56
CAS:	19781-72-7

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
tb	733.75	K	Joback Method
tc	904.73	K	Joback Method
tf	337.00 ± 0.10	K	NIST Webbook
vc	1.218	m3/kmol	Joback Method

Temperature Dependent Properties

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

cpg	1044.00	J/mol×K	904.73	Joback Method
dvisc	0.0022413	Pa×s	376.36	Joback Method
dvisc	0.0000844	Pa×s	733.75	Joback Method
dvisc	0.0001145	Pa×s	674.18	Joback Method
dvisc	0.0001648	Pa×s	614.62	Joback Method
dvisc	0.0002565	Pa×s	555.06	Joback Method
dvisc	0.0004441	Pa×s	495.49	Joback Method
dvisc	0.0008932	Pa×s	435.93	Joback Method
hfust	76.20	kJ/mol	336.70	NIST Webbook
hfust	76.20	kJ/mol	336.70	NIST Webbook

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=C19781727&Units=SI

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
hfust: Enthalpy of fusion at a given temperature
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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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