Behenic alcohol

Other names:	1-Docosanol
	Abreva
	Behenyl alcohol
	Cachalot BE-22
	Dehydag wax 22 (lanette)
	Docosan-1-ol
	Docosanol
	Docosanol-(1)
	Docosyl alcohol
	Emery 3304
	IK 2
	Lanette 22
	Loxiol VPG 1451
	N-Eicosanol
	NAA 422
	NSC 8407
	Nacol 22-97
	Stenol 1822
	Stenol 1822A
	Tadenan
	n-Docosanol
Inchi:	InChI=1S/C22H46O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23/h23
InchiKey:	NOPFSRXAKWQILS-UHFFFAOYSA-N
Formula:	C22H46O
SMILES:	CCCCCCCCCCCCCCCCCCCCCCO
Mol. weight [g/mol]:	326.60
CAS:	661-19-8

Physical Properties

Property code	Value	Unit	Source
chl	-14450.00 ± 10.00	kJ/mol	NIST Webbook
gf	-2.46	kJ/mol	Joback Method
hf	-649.64	kJ/mol	Joback Method
hfus	56.82	kJ/mol	Joback Method
hsub	207.00 ± 10.00	kJ/mol	NIST Webbook
hsub	239.00 ± 10.00	kJ/mol	NIST Webbook

hvap	135.90 ± 0.80	kJ/mol	NIST Webbook
log10ws	-8.29		Crippen Method
logp	7.801		Crippen Method
mcvol	326.710	ml/mol	McGowan Method
pc	953.78	kPa	Joback Method
rinpol	2468.00		NIST Webbook
rinpol	2473.00		NIST Webbook
rinpol	2498.00		NIST Webbook
rinpol	2456.00		NIST Webbook
rinpol	397.16		NIST Webbook
rinpol	401.29		NIST Webbook
rinpol	2476.00		NIST Webbook
rinpol	400.57		NIST Webbook
rinpol	367.90		NIST Webbook
rinpol	2470.40		NIST Webbook
rinpol	2475.00		NIST Webbook
rinpol	2470.40		NIST Webbook
rinpol	2456.00		NIST Webbook
rinpol	2501.00		NIST Webbook
rinpol	2501.40		NIST Webbook
rinpol	2470.00		NIST Webbook
rinpol	2456.00		NIST Webbook
rinpol	2493.00		NIST Webbook
rinpol	2470.00		NIST Webbook
rinpol	2494.00		NIST Webbook
rinpol	2443.00		NIST Webbook
rinpol	2497.00		NIST Webbook
rinpol	2467.00		NIST Webbook
rinpol	2456.00		NIST Webbook
rinpol	2501.40		NIST Webbook
ripol	2979.00		NIST Webbook
ripol	2979.00		NIST Webbook
tb	794.94	K	Joback Method
tc	973.24	K	Joback Method
tf	344.50	K	Evaluation of the Vaporization, Fusion, and Sublimation Enthalpies of the 1-Alkanols: The Vaporization Enthalpy of 1-, 6-, 7-, and 9-Heptadecanol, 1-Octadecanol, 1-Eicosanol, 1-Docosanol, 1-Hexacosanol, and Cholesterol at T) 298.15 K by Correlation Gas Chromatography
tf	343.20 ± 3.00	K	NIST Webbook

tf	342.40 ± 0.60	K	NIST Webbook
tf	343.00 ± 0.25	K	NIST Webbook
vc	1.286	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1050.02	J/mol×K	794.94	Joback Method
cpg	1159.25	J/mol×K	973.24	Joback Method
cpg	1090.11	J/mol×K	854.37	Joback Method
cpg	1108.71	J/mol×K	884.09	Joback Method
cpg	1126.41	J/mol×K	913.81	Joback Method
cpg	1143.24	J/mol×K	943.52	Joback Method
cpg	1070.56	J/mol×K	824.66	Joback Method
dvisc	0.0000216	Pa×s	728.87	Joback Method
dvisc	0.0000379	Pa×s	662.80	Joback Method
dvisc	0.0000752	Pa×s	596.73	Joback Method
dvisc	0.0001770	Pa×s	530.66	Joback Method
dvisc	0.0005314	Pa×s	464.59	Joback Method
dvisc	0.0000136	Pa×s	794.94	Joback Method
dvisc	0.0022967	Pa×s	398.52	Joback Method
hfust	86.06	kJ/mol	343.90	NIST Webbook
hfust	85.07	kJ/mol	240.00	NIST Webbook
hfust	46.57	kJ/mol	345.20	NIST Webbook
hfust	17.24	kJ/mol	333.90	NIST Webbook
hfust	46.57	kJ/mol	345.20	NIST Webbook
hsubt	207.00 ± 10.00	kJ/mol	338.00	NIST Webbook
hvapt	115.30	kJ/mol	401.50	NIST Webbook
sfust	50.72	J/mol×K	333.90	NIST Webbook
sfust	134.90	J/mol×K	345.20	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	453.20	K	0.03	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.51940e+01
Coeff. B	-5.76455e+03
Coeff. C	-1.22684e+02
Temperature range (K), min.	509.40
Temperature range (K), max.	705.99

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Phase equilibria of high molecular mass 1-alcohols in supercritical propane:	https://www.doi.org/10.1016/j.fluid.2007.04.027
Evaluation of the Vaporization, Fusion, and Sublimation Enthalpies of the 1-Alkanols: The Vaporization Enthalpy of 1-, 6-, 7- and 9-Heptadecanol, 1-Octadecanol, 1-Eicosanol, 1-Docosanol, 1-Hexacosanol, and Cholesterol at T) 298.15 K by Correlation Gas Chromatography:	https://www.doi.org/10.1021/je0503857
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=C661198&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

chl:	Standard liquid enthalpy of combustion
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
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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