Behenyl chloride

Other names:	1-Chlorodocosane
	Docosane, 1-chloro-
Inchi:	InChI=1S/C22H45Cl/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23/h2-
InchiKey:	OACXFSZVCDOBKF-UHFFFAOYSA-N
Formula:	C22H45Cl
SMILES:	CCCCCCCCCCCCCCCCCCCCCCCCCl
Mol. weight [g/mol]:	345.05
CAS:	42217-03-8

Physical Properties

Property code	Value	Unit	Source
gf	122.43	kJ/mol	Joback Method
hf	-513.15	kJ/mol	Joback Method
hfus	56.93	kJ/mol	Joback Method
hvap	68.95	kJ/mol	Joback Method
log10ws	-9.18		Crippen Method
logp	9.047		Crippen Method
mcvol	333.080	ml/mol	McGowan Method
pc	882.09	kPa	Joback Method
ripol	2692.00		NIST Webbook
tb	740.19	K	Joback Method
tc	910.35	K	Joback Method
tf	367.62	K	Joback Method
vc	1.317	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1002.07	J/mol×K	740.19	Joback Method
cpg	1023.16	J/mol×K	768.55	Joback Method
cpg	1043.28	J/mol×K	796.91	Joback Method
cpg	1062.48	J/mol×K	825.27	Joback Method
cpg	1080.80	J/mol×K	853.63	Joback Method
cpg	1098.27	J/mol×K	881.99	Joback Method

cpg	1114.92	J/mol×K	910.35	Joback Method
dvisc	0.0021878	Pa×s	367.62	Joback Method
dvisc	0.0008019	Pa×s	429.71	Joback Method
dvisc	0.0003787	Pa×s	491.81	Joback Method
dvisc	0.0002116	Pa×s	553.90	Joback Method
dvisc	0.0001330	Pa×s	616.00	Joback Method
dvisc	0.0000910	Pa×s	678.10	Joback Method
dvisc	0.0000663	Pa×s	740.19	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.32945e+01
Coeff. B	-5.05479e+03
Coeff. C	-1.26896e+02
Temperature range (K), min.	515.52
Temperature range (K), max.	760.09

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C42217038&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume