1-Bromodocosane

Other names: Behenyl bromide
Docosane, 1-bromo-
n-Docosyl bromide
Inchi: InChI=1S/C22H45Br/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: QYOXLKAKUAASNA-UHFFFAOYSA-N
Formula: C22H45Br
SMILES: CCCCCCCCCCCCCCCCCCCCCCBr
Mol. weight [g/mol]: 389.50
CAS: 6938-66-5

Physical Properties

Property code	Value	Unit	Source
gf	148.68	kJ/mol	Joback Method
hf	-471.08	kJ/mol	Joback Method
hfus	58.02	kJ/mol	Joback Method
hvap	71.00	kJ/mol	Joback Method
log10ws	-9.46		Crippen Method
logp	9.203		Crippen Method
mcvol	338.340	ml/mol	McGowan Method
pc	940.37	kPa	Joback Method
tb	768.92	K	Joback Method
tc	945.29	K	Joback Method
tf	317.00	K	NIST Webbook
tf	313.20 ± 0.60	K	NIST Webbook
vc	1.329	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1024.13	J/mol×K	768.92	Joback Method
cpg	1044.89	J/mol×K	798.32	Joback Method
cpg	1064.68	J/mol×K	827.71	Joback Method
cpg	1083.54	J/mol×K	857.11	Joback Method
cpg	1101.51	J/mol×K	886.50	Joback Method

cpg	1118.65	J/mol×K	915.90	Joback Method
cpg	1134.98	J/mol×K	945.29	Joback Method
dvisc	0.0015580	Pa×s	397.50	Joback Method
dvisc	0.0006309	Pa×s	459.40	Joback Method
dvisc	0.0003167	Pa×s	521.31	Joback Method
dvisc	0.0001840	Pa×s	583.21	Joback Method
dvisc	0.0001186	Pa×s	645.11	Joback Method
dvisc	0.0000826	Pa×s	707.02	Joback Method
dvisc	0.0000610	Pa×s	768.92	Joback Method
hfust	44.98	kJ/mol	317.10	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	498.00	K	0.08	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48265e+01
Coeff. B	-5.73428e+03
Coeff. C	-1.30510e+02
Temperature range (K), min.	524.92
Temperature range (K), max.	733.17

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6938665&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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume