1-Bromoeicosane

Other names:	EICOSYL BROMIDE
	Eicosane, 1-bromo-
	N-EICOSYL BROMIDE
	bromoicosane
Inchi:	InChI=1S/C20H41Br/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21/h2-20H2,
InchiKey:	CZASMUMJSKOHFJ-UHFFFAOYSA-N
Formula:	C20H41Br
SMILES:	CCCCCCCCCCCCCCCCCCCCBr
Mol. weight [g/mol]:	361.44
CAS:	4276-49-7

Physical Properties

Property code	Value	Unit	Source
gf	131.84	kJ/mol	Joback Method
hf	-429.80	kJ/mol	Joback Method
hfus	52.84	kJ/mol	Joback Method
hvap	66.55	kJ/mol	Joback Method
log10ws	-8.63		Crippen Method
logp	8.423		Crippen Method
mcvol	310.160	ml/mol	McGowan Method
pc	1061.71	kPa	Joback Method
rinpol	2364.00		NIST Webbook
tb	723.16	K	Joback Method
tc	895.45	K	Joback Method
tf	309.75 ± 1.00	K	NIST Webbook
vc	1.218	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	902.08	J/mol×K	723.16	Joback Method
cpg	921.98	J/mol×K	751.88	Joback Method
cpg	940.97	J/mol×K	780.59	Joback Method
cpg	959.09	J/mol×K	809.31	Joback Method

cpg	976.39	J/mol×K	838.02	Joback Method
cpg	992.90	J/mol×K	866.74	Joback Method
cpg	1008.65	J/mol×K	895.45	Joback Method
dvisc	0.0019498	Pa×s	374.96	Joback Method
dvisc	0.0008040	Pa×s	432.99	Joback Method
dvisc	0.0004087	Pa×s	491.03	Joback Method
dvisc	0.0002397	Pa×s	549.06	Joback Method
dvisc	0.0001557	Pa×s	607.09	Joback Method
dvisc	0.0001091	Pa×s	665.13	Joback Method
dvisc	0.0000809	Pa×s	723.16	Joback Method
hvapt	79.80	kJ/mol	587.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50893e+01
Coeff. B	-5.66795e+03
Coeff. C	-1.24394e+02
Temperature range (K), min.	507.32
Temperature range (K), max.	704.07

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

KDB: https://www.cheric.org/files/research/kdb/mol/mol1659.mol

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4276497&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

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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume