

Octadecane, 1-bromo-

Other names:	1-Bromooctadecane N-OCTADECYL BROMIDE Octadecyl bromide STEARYL BROMIDE
Inchi:	InChI=1S/C18H37Br/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19/h2-18H2,1H3
InchiKey:	WSULSMOGMLRGKU-UHFFFAOYSA-N
Formula:	C18H37Br
SMILES:	CCCCCCCCCCCCCCCCCBr
Mol. weight [g/mol]:	333.39
CAS:	112-89-0

Physical Properties

Property code	Value	Unit	Source
gf	115.00	kJ/mol	Joback Method
hf	-388.52	kJ/mol	Joback Method
hfus	47.66	kJ/mol	Joback Method
hvap	62.10	kJ/mol	Joback Method
log10ws	-7.79		Crippen Method
logp	7.643		Crippen Method
mcvol	281.980	ml/mol	McGowan Method
pc	1208.15	kPa	Joback Method
rinpol	2172.00		NIST Webbook
rinpol	2161.00		NIST Webbook
rinpol	2172.00		NIST Webbook
rinpol	2161.00		NIST Webbook
rinpol	2180.00		NIST Webbook
rinpol	2180.00		NIST Webbook
ripol	2447.00		

tf	296.65	K	Fabrication and properties of poly(polyethylene glycol n-alkyl ether vinyl ether)s as polymeric phase change materials
tf	303.00 ± 3.00	K	NIST Webbook
vc	1.105	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	784.07	J/mol×K	677.40	Joback Method
cpg	803.16	J/mol×K	705.82	Joback Method
cpg	821.41	J/mol×K	734.24	Joback Method
cpg	838.85	J/mol×K	762.66	Joback Method
cpg	855.50	J/mol×K	791.07	Joback Method
cpg	871.41	J/mol×K	819.49	Joback Method
cpg	886.59	J/mol×K	847.91	Joback Method
dvisc	0.0023948	Pa×s	352.42	Joback Method
dvisc	0.0010077	Pa×s	406.58	Joback Method
dvisc	0.0005197	Pa×s	460.75	Joback Method
dvisc	0.0003081	Pa×s	514.91	Joback Method
dvisc	0.0002018	Pa×s	569.07	Joback Method
dvisc	0.0001422	Pa×s	623.24	Joback Method
dvisc	0.0001060	Pa×s	677.40	Joback Method
hvapt	81.00			

Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.53450e+01
Coeff. B	-5.57724e+03
Coeff. C	-1.17722e+02
Temperature range (K), min.	488.12
Temperature range (K), max.	673.58

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Fabrication and properties of poly(polyethylene glycol n-alkyl ether) Joback Method:	https://www.doi.org/10.1016/j.tca.2016.04.007
Joback Method: polymeric phase change materials:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.therc.org/files/research/kdb/mol/mol1657.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C112890&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

vc: Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/73-830-9/Octadecane-1-bromo.pdf>

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