1-Bromotridecane

Other names: Tridecyl bromide
n-Tridecyl bromide
n-Tridecyl-1-bromide
Inchi: InChI=1S/C13H27Br/c1-2-3-4-5-6-7-8-9-10-11-12-13-14/h2-13H2,1H3
InchiKey: BFDNZQUBFCYTIC-UHFFFAOYSA-N
Formula: C13H27Br
SMILES: CCCCCCCCCCCCCBr
Mol. weight [g/mol]: 263.26
CAS: 765-09-3

Physical Properties

Property code	Value	Unit	Source
af	0.7235		Cheméo Relay (1.0)
gf	72.90	kJ/mol	Joback Method
hf	-311.52	kJ/mol	Cheméo Relay (1.0)
hfus	34.71	kJ/mol	Joback Method
hvap	79.66	kJ/mol	Cheméo Relay (1.0)
ie	9.85	eV	Cheméo Relay (1.0)
log10ws	-6.88		Cheméo Relay (1.0)
logp	5.692		Crippen Method
mcvol	211.530	ml/mol	McGowan Method
pc	1740.46	kPa	Joback Method
rinpol	1658.00		NIST Webbook
rinpol	1658.00		NIST Webbook
rinpol	1651.00		NIST Webbook
rinpol	1652.00		NIST Webbook
rinpol	1652.00		NIST Webbook
rinpol	1651.00		NIST Webbook
ripol	1905.00		NIST Webbook
ripol	1900.00		NIST Webbook
tb	556.52	K	Cheméo Relay (1.0)
tc	726.87	K	Cheméo Relay (1.0)
tf	279.10 ± 0.30	K	NIST Webbook
vc	0.834	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	510.67	J/mol×K	563.00	Joback Method
cpg	601.20	J/mol×K	736.25	Joback Method
cpg	587.77	J/mol×K	707.38	Joback Method
cpg	573.71	J/mol×K	678.50	Joback Method
cpg	559.00	J/mol×K	649.63	Joback Method
cpg	543.61	J/mol×K	620.75	Joback Method
cpg	527.50	J/mol×K	591.88	Joback Method
dvisc	0.0005323	Pa×s	429.54	Joback Method
dvisc	0.0001950	Pa×s	563.00	Joback Method
dvisc	0.0002573	Pa×s	518.51	Joback Method
dvisc	0.0003577	Pa×s	474.02	Joback Method
dvisc	0.0035921	Pa×s	296.07	Joback Method
dvisc	0.0008683	Pa×s	385.05	Joback Method
dvisc	0.0016097	Pa×s	340.56	Joback Method
hvapt	64.60	kJ/mol	526.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	422.20	K	1.30	NIST Webbook
tbrp	421.00	K	1.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.59689e+01
Coeff. B	-5.23534e+03
Coeff. C	-9.82620e+01
Temperature range (K), min.	432.12
Temperature range (K), max.	589.50

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C765093&Units=SI

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume