2-Bromo dodecane

Other names: 2-bromododecane
Dodecane, 2-bromo-
Inchi: InChI=1S/C12H25Br/c1-3-4-5-6-7-8-9-10-11-12(2)13/h12H,3-11H2,1-2H3
InchiKey: GIUUCQVKMWBSRT-UHFFFAOYSA-N
Formula: C12H25Br
SMILES: CCCCCCCCCCC(C)Br
Mol. weight [g/mol]: 249.23
CAS: 13187-99-0

Physical Properties

Property code	Value	Unit	Source
gf	62.04	kJ/mol	Joback Method
hf	-269.96	kJ/mol	Joback Method
hfus	28.60	kJ/mol	Joback Method
hvap	48.35	kJ/mol	Joback Method
log10ws	-5.39		Crippen Method
logp	5.301		Crippen Method
mcvol	197.440	ml/mol	McGowan Method
pc	1901.92	kPa	Joback Method
rinpol	1505.00		NIST Webbook
ripol	1702.00		NIST Webbook
ripol	1702.00		NIST Webbook
tb	539.68	K	Joback Method
tc	717.63	K	Joback Method
tf	269.80	K	Joback Method
vc	0.763	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	460.64	J/mol×K	539.68	Joback Method
cpg	477.25	J/mol×K	569.34	Joback Method
cpg	493.12	J/mol×K	599.00	Joback Method
cpg	508.27	J/mol×K	628.65	Joback Method

cpg	522.73	J/mol×K	658.31	Joback Method
cpg	536.53	J/mol×K	687.97	Joback Method
cpg	549.69	J/mol×K	717.63	Joback Method
dvisc	0.0053574	Pa×s	269.80	Joback Method
dvisc	0.0021059	Pa×s	314.78	Joback Method
dvisc	0.0010455	Pa×s	359.76	Joback Method
dvisc	0.0006065	Pa×s	404.74	Joback Method
dvisc	0.0003923	Pa×s	449.72	Joback Method
dvisc	0.0002747	Pa×s	494.70	Joback Method
dvisc	0.0002041	Pa×s	539.68	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	400.50 ± 2.50	K	1.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.52116e+01
Coeff. B	-4.77916e+03
Coeff. C	-9.10060e+01
Temperature range (K), min.	411.24
Temperature range (K), max.	573.75

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13187990&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

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
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