Tridecane, 2-bromo-

Other names: 2-Bromotridecane
Inchi: InChI=1S/C13H27Br/c1-3-4-5-6-7-8-9-10-11-12-13(2)14/h13H,3-12H2,1-2H3
InchiKey: XNCUZDYTCKIDEJ-UHFFFAOYSA-N
Formula: C13H27Br
SMILES: CCCCCCCCCCCC(C)Br
Mol. weight [g/mol]: 263.26
CAS: 59157-17-4

Physical Properties

Property code	Value	Unit	Source
gf	70.46	kJ/mol	Joback Method
hf	-290.60	kJ/mol	Joback Method
hfus	31.19	kJ/mol	Joback Method
hvap	50.58	kJ/mol	Joback Method
log10ws	-5.81		Crippen Method
logp	5.691		Crippen Method
mcvol	211.530	ml/mol	McGowan Method
pc	1752.14	kPa	Joback Method
rinpol	1609.00		NIST Webbook
rinpol	1609.00		NIST Webbook
tb	562.56	K	Joback Method
tc	738.95	K	Joback Method
tf	281.07	K	Joback Method
vc	0.820	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	510.95	J/mol×K	562.56	Joback Method
cpg	528.15	J/mol×K	591.96	Joback Method
cpg	544.58	J/mol×K	621.36	Joback Method
cpg	560.27	J/mol×K	650.75	Joback Method
cpg	575.24	J/mol×K	680.15	Joback Method
cpg	589.53	J/mol×K	709.55	Joback Method

cpg	603.16	J/mol×K	738.95	Joback Method
dvisc	0.0049890	Pa×s	281.07	Joback Method
dvisc	0.0019389	Pa×s	327.99	Joback Method
dvisc	0.0009546	Pa×s	374.90	Joback Method
dvisc	0.0005502	Pa×s	421.81	Joback Method
dvisc	0.0003541	Pa×s	468.73	Joback Method
dvisc	0.0002470	Pa×s	515.64	Joback Method
dvisc	0.0001829	Pa×s	562.56	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.51312e+01
Coeff. B	-4.87818e+03
Coeff. C	-9.54820e+01
Temperature range (K), min.	424.12
Temperature range (K), max.	592.26

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C59157174&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

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

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