1,14-dibromotetradecane

Inchi: InChI=1S/C14H28Br2/c15-13-11-9-7-5-3-1-2-4-6-8-10-12-14-16/h1-14H2
InchiKey: SDENLXLNLFKRAR-UHFFFAOYSA-N
Formula: C14H28Br2
SMILES: BrCCCCCCCCCCCCCCBr
Mol. weight [g/mol]: 356.19
CAS: 37688-96-3

Physical Properties

Property code	Value	Unit	Source
af	0.8639		Cheméo Relay (1.0)
gf	95.64	kJ/mol	Joback Method
hf	-318.89	kJ/mol	Cheméo Relay (1.0)
hfus	42.59	kJ/mol	Joback Method
hvap	98.48	kJ/mol	Cheméo Relay (1.0)
ie	9.94	eV	Cheméo Relay (1.0)
log10ws	-7.43		Cheméo Relay (1.0)
logp	6.457		Crippen Method
mcvol	243.120	ml/mol	McGowan Method
pc	1701.90	kPa	Joback Method
tb	587.38	K	Cheméo Relay (1.0)
tc	768.82	K	Cheméo Relay (1.0)
tf	322.39	K	Cheméo Relay (1.0)
vc	0.936	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	613.64	J/mol×K	652.04	Joback Method
cpg	700.56	J/mol×K	835.72	Joback Method
cpg	687.79	J/mol×K	805.11	Joback Method
cpg	674.39	J/mol×K	774.50	Joback Method
cpg	660.32	J/mol×K	743.88	Joback Method
cpg	645.53	J/mol×K	713.27	Joback Method
cpg	629.98	J/mol×K	682.65	Joback Method

dvisc	0.0003802	Pa×s	509.59	Joback Method
dvisc	0.0001482	Pa×s	652.04	Joback Method
dvisc	0.0001931	Pa×s	604.56	Joback Method
dvisc	0.0002632	Pa×s	557.07	Joback Method
dvisc	0.0020272	Pa×s	367.14	Joback Method
dvisc	0.0005923	Pa×s	462.11	Joback Method
dvisc	0.0010212	Pa×s	414.62	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.74259e+01
Coeff. B	-6.27642e+03
Coeff. C	-1.15498e+02
Temperature range (K), min.	481.72
Temperature range (K), max.	633.59

Sources

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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):

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