2-bromodecane

Inchi: InChI=1S/C10H21Br/c1-3-4-5-6-7-8-9-10(2)11/h10H,3-9H2,1-2H3
InchiKey: HRDKIHSQGRCTMR-UHFFFAOYSA-N
Formula: C10H21Br
SMILES: CCCCCCCCC(C)Br
Mol. weight [g/mol]: 221.18
CAS: 39563-53-6

Physical Properties

Property code	Value	Unit	Source
gf	45.20	kJ/mol	Joback Method
hf	-228.68	kJ/mol	Joback Method
hfus	23.42	kJ/mol	Joback Method
hvap	43.90	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	4.520		Crippen Method
mcvol	169.260	ml/mol	McGowan Method
pc	2265.42	kPa	Joback Method
ripol	1493.00		NIST Webbook
ripol	1493.00		NIST Webbook
tb	493.92	K	Joback Method
tc	675.34	K	Joback Method
tf	247.26	K	Joback Method
vc	0.651	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	365.14	J/mol×K	493.92	Joback Method
cpg	434.51	J/mol×K	645.10	Joback Method
cpg	421.91	J/mol×K	614.87	Joback Method
cpg	408.69	J/mol×K	584.63	Joback Method
cpg	394.84	J/mol×K	554.39	Joback Method
cpg	380.33	J/mol×K	524.16	Joback Method
cpg	446.53	J/mol×K	675.34	Joback Method

dvisc	0.0002493	Pa×s	493.92	Joback Method
dvisc	0.0003329	Pa×s	452.81	Joback Method
dvisc	0.0004712	Pa×s	411.70	Joback Method
dvisc	0.0007202	Pa×s	370.59	Joback Method
dvisc	0.0012237	Pa×s	329.48	Joback Method
dvisc	0.0024187	Pa×s	288.37	Joback Method
dvisc	0.0059960	Pa×s	247.26	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53048e+01
Coeff. B	-4.53230e+03
Coeff. C	-8.11920e+01
Temperature range (K), min.	383.00
Temperature range (K), max.	534.73

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C39563536&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

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