1,2,3-tribromobutane

Inchi: InChI=1S/C4H7Br3/c1-3(6)4(7)2-5/h3-4H,2H2,1H3
InchiKey: HKTNRDJXZCCMGH-UHFFFAOYSA-N
Formula: C4H7Br3
SMILES: CC(Br)C(Br)CBr
Mol. weight [g/mol]: 294.81
CAS: 632-05-3

Physical Properties

Property code	Value	Unit	Source
gf	20.88	kJ/mol	Joback Method
hf	-57.46	kJ/mol	Joback Method
hfus	14.92	kJ/mol	Joback Method
hvap	43.03	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	2.928		Crippen Method
mcvol	119.720	ml/mol	McGowan Method
pc	5258.62	kPa	Joback Method
tb	488.52	K	Joback Method
tc	723.92	K	Joback Method
tf	284.24	K	Joback Method
vc	0.433	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	219.73	J/mol×K	684.68	Joback Method
cpg	214.17	J/mol×K	645.45	Joback Method
cpg	208.15	J/mol×K	606.22	Joback Method
cpg	201.63	J/mol×K	566.99	Joback Method
cpg	194.55	J/mol×K	527.75	Joback Method
cpg	186.87	J/mol×K	488.52	Joback Method
cpg	224.89	J/mol×K	723.92	Joback Method
dvisc	0.0041502	Pa×s	284.24	Joback Method
dvisc	0.0003845	Pa×s	488.52	Joback Method

dvisc	0.0004927	Pa×s	454.47	Joback Method
dvisc	0.0006573	Pa×s	420.43	Joback Method
dvisc	0.0009224	Pa×s	386.38	Joback Method
dvisc	0.0013822	Pa×s	352.33	Joback Method
dvisc	0.0022583	Pa×s	318.29	Joback Method
hvapt	54.10	kJ/mol	470.00	NIST Webbook
hvapt	51.30	kJ/mol	403.50	NIST Webbook

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=C632053&Units=SI
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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume