1,3,5-tris-(Bromomethyl) cyclohexane

Inchi: InChI=1S/C9H15Br3/c10-4-7-1-8(5-11)3-9(2-7)6-12/h7-9H,1-6H2
InchiKey: HPDNDWLWKJEJTR-UHFFFAOYSA-N
Formula: C9H15Br3
SMILES: BrCC1CC(CBr)CC(CBr)C1
Mol. weight [g/mol]: 362.93

Physical Properties

Property code	Value	Unit	Source
gf	76.89	kJ/mol	Joback Method
hf	-136.46	kJ/mol	Joback Method
hfus	28.90	kJ/mol	Joback Method
hvap	54.74	kJ/mol	Joback Method
log10ws	-4.05		Crippen Method
logp	4.204		Crippen Method
mcvol	179.310	ml/mol	McGowan Method
pc	3318.18	kPa	Joback Method
rinpol	1937.00		NIST Webbook
rinpol	1937.00		NIST Webbook
tb	614.01	K	Joback Method
tc	858.93	K	Joback Method
tf	369.49	K	Joback Method
vc	0.656	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	395.57	J/mol×K	614.01	Joback Method
cpg	411.92	J/mol×K	654.83	Joback Method
cpg	427.09	J/mol×K	695.65	Joback Method
cpg	441.14	J/mol×K	736.47	Joback Method
cpg	454.14	J/mol×K	777.29	Joback Method
cpg	466.15	J/mol×K	818.11	Joback Method
cpg	477.24	J/mol×K	858.93	Joback Method
dvisc	0.0019928	Pa×s	369.49	Joback Method

dvisc	0.0012818	Pa×s	410.24	Joback Method
dvisc	0.0008930	Pa×s	451.00	Joback Method
dvisc	0.0006605	Pa×s	491.75	Joback Method
dvisc	0.0005116	Pa×s	532.50	Joback Method
dvisc	0.0004110	Pa×s	573.26	Joback Method
dvisc	0.0003398	Pa×s	614.01	Joback Method

Sources

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=R96333&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume