

1,3-bis-(Bromomethyl)-5-hydroxymethylcyclohexane

Inchi:
acetate

InChI=1S/C11H18Br2O2/c1-8(14)15-7-11-3-9(5-12)2-10(4-11)6-13/h9-11H,2-7H2,1H3

InchiKey:

XIWIVBCWZGLHNO-UHFFFAOYSA-N

Formula:

C11H18Br2O2

SMILES:

CC(=O)OCC1CC(CBr)CC(CBr)C1

Mol. weight [g/mol]:

342.07

Physical Properties

Property code	Value	Unit	Source
gf	-154.51	kJ/mol	Joback Method
hf	-448.87	kJ/mol	Joback Method
hfus	31.58	kJ/mol	Joback Method
hvap	61.92	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	3.372		Crippen Method
mcvol	197.430	ml/mol	McGowan Method
pc	2627.15	kPa	Joback Method
rinsol	1955.00		NIST Webbook
tb	669.90	K	Joback Method
tc	896.46	K	Joback Method
tf	404.39	K	Joback Method
vc	0.731	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	500.24	J/molxK	669.90	Joback Method
cpg	573.20	J/molxK	858.70	Joback Method
cpg	560.75	J/molxK	820.94	Joback Method
cpg	547.26	J/molxK	783.18	Joback Method
cpg	532.69	J/molxK	745.42	Joback Method
cpg	517.03	J/molxK	707.66	Joback Method
cpg	584.62	J/molxK	896.46	Joback Method
dvisc	0.0002534	Paxs	669.90	Joback Method
dvisc	0.0003101	Paxs	625.65	Joback Method

dvisc	0.0003914	Paxs	581.40	Joback Method
dvisc	0.0005133	Paxs	537.14	Joback Method
dvisc	0.0007067	Paxs	492.89	Joback Method
dvisc	0.0010362	Paxs	448.64	Joback Method
dvisc	0.0016523	Paxs	404.39	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=R96383&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

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