1-Bromomethyl-3,5-bis-(Hydroxymethyl)cyclohexa diacetate

InChI: InChI=1S/C13H21BrO4/c1-9(15)17-7-12-3-11(6-14)4-13(5-12)8-18-10(2)16/h11-13H,3-8
InChIKey: QFBQQXCSNNKORI-UHFFFAOYSA-N
Formula: C13H21BrO4
SMILES: CC(=O)OCC1CC(CBr)CC(COC(C)=O)C1
Mol. weight [g/mol]: 321.21

Physical Properties

Property code	Value	Unit	Source
gf	-385.91	kJ/mol	Joback Method
hf	-761.28	kJ/mol	Joback Method
hfus	34.26	kJ/mol	Joback Method
hvap	69.09	kJ/mol	Joback Method
log10ws	-2.59		Crippen Method
logp	2.540		Crippen Method
mcvol	215.550	ml/mol	McGowan Method
pc	2131.49	kPa	Joback Method
rinpol	1974.00		NIST Webbook
tb	725.79	K	Joback Method
tc	938.32	K	Joback Method
tf	439.29	K	Joback Method
vc	0.804	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	611.81	J/mol×K	725.79	Joback Method
cpg	684.72	J/mol×K	902.90	Joback Method
cpg	672.44	J/mol×K	867.48	Joback Method
cpg	659.00	J/mol×K	832.05	Joback Method
cpg	644.42	J/mol×K	796.63	Joback Method
cpg	628.69	J/mol×K	761.21	Joback Method
cpg	695.86	J/mol×K	938.32	Joback Method
dvisc	0.0001831	Pa×s	725.79	Joback Method
dvisc	0.0002263	Pa×s	678.04	Joback Method

dvisc	0.0002888	Pa×s	630.29	Joback Method
dvisc	0.0003838	Pa×s	582.54	Joback Method
dvisc	0.0005364	Pa×s	534.79	Joback Method
dvisc	0.0008006	Pa×s	487.04	Joback Method
dvisc	0.0013037	Pa×s	439.29	Joback Method

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=R96397&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
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