Diethylene glycol bis-bromoacetate

Inchi: InChI=1S/C8H12Br2O5/c9-5-7(11)14-3-1-13-2-4-15-8(12)6-10/h1-6H2
InchiKey: ODNPUMPXGXZVLR-UHFFFAOYSA-N
Formula: C8H12Br2O5
SMILES: O=C(CBr)OCCOCCOC(=O)CBr
Mol. weight [g/mol]: 347.99
CAS: 90783-54-3

Physical Properties

Property code	Value	Unit	Source
gf	-527.72	kJ/mol	Joback Method
hf	-777.61	kJ/mol	Joback Method
hfus	33.81	kJ/mol	Joback Method
hvap	66.99	kJ/mol	Joback Method
log10ws	-0.85		Crippen Method
logp	0.879		Crippen Method
mcvol	179.330	ml/mol	McGowan Method
pc	3181.14	kPa	Joback Method
tb	689.76	K	Joback Method
tc	895.67	K	Joback Method
tf	466.07	K	Joback Method
vc	0.673	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	415.96	J/mol×K	689.76	Joback Method
cpg	459.66	J/mol×K	861.35	Joback Method
cpg	452.12	J/mol×K	827.03	Joback Method
cpg	443.98	J/mol×K	792.71	Joback Method
cpg	435.23	J/mol×K	758.40	Joback Method
cpg	425.89	J/mol×K	724.08	Joback Method
cpg	466.57	J/mol×K	895.67	Joback Method
dvisc	0.0001412	Pa×s	689.76	Joback Method
dvisc	0.0001736	Pa×s	652.48	Joback Method

dvisc	0.0002188	Pa×s	615.20	Joback Method
dvisc	0.0002842	Pa×s	577.91	Joback Method
dvisc	0.0003826	Pa×s	540.63	Joback Method
dvisc	0.0005383	Pa×s	503.35	Joback Method
dvisc	0.0007998	Pa×s	466.07	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=C90783543&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume