7-Oxabicyclo[2.2.1]heptane-2,3-dicarboxylic acid

Other names: 1,2-Benzenedicarboxylic acid, hexahydro-3,6-endo-oxy-
1,2-Cyclohexanedicarboxylic acid, 3,6-endo-epoxy-
3,6-Endoxohexahydrophthalic acid
3,6-endo-Oxohexahydrophthalic acid
3,6-endo-Oxyphthalic acid hexahydro-
62059-43-2 (hydrate)
Aquathol
Aquothol
Endothal
Endothal technical
Endothall
Endothall weed killer
Herbon pennout
Hydout
Hydrothal-191
Hydrothal-47
Hydrothol
NSC 112771
Niagrathal
Phthalic acid, hexahydro-3,6-endo-oxy-
Rcra waste number P088
Tri-Endothal

Inchi: InChI=1S/C8H10O5/c9-7(10)5-3-1-2-4(13-3)6(5)8(11)12/h3-6H,1-2H2,(H,9,10)(H,11,12)

InchiKey: GXEKYRXVRROBEV-UHFFFAOYSA-N

Formula: C8H10O5

SMILES: O=C(O)C1C2CCC(O2)C1C(=O)O

Mol. weight [g/mol]: 186.16

CAS: 145-73-3

Physical Properties

Property code	Value	Unit	Source
gf	-507.14	kJ/mol	Joback Method
hf	-771.31	kJ/mol	Joback Method
hfus	32.14	kJ/mol	Joback Method
hvap	84.14	kJ/mol	Joback Method
log10ws	-0.27		Aqueous Solubility Prediction Method

logp	-0.051		Crippen Method
mcvol	122.610	ml/mol	McGowan Method
pc	4652.99	kPa	Joback Method
tb	709.90	K	Joback Method
tc	904.89	K	Joback Method
tf	451.87	K	Joback Method
vc	0.459	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	375.75	J/mol×K	709.90	Joback Method
cpg	385.13	J/mol×K	742.40	Joback Method
cpg	393.92	J/mol×K	774.90	Joback Method
cpg	402.14	J/mol×K	807.40	Joback Method
cpg	409.84	J/mol×K	839.89	Joback Method
cpg	417.07	J/mol×K	872.39	Joback Method
cpg	423.85	J/mol×K	904.89	Joback Method
dvisc	0.0033970	Pa×s	451.87	Joback Method
dvisc	0.0016020	Pa×s	494.88	Joback Method
dvisc	0.0008520	Pa×s	537.88	Joback Method
dvisc	0.0004975	Pa×s	580.88	Joback Method
dvisc	0.0003129	Pa×s	623.89	Joback Method
dvisc	0.0002089	Pa×s	666.89	Joback Method
dvisc	0.0001465	Pa×s	709.90	Joback Method

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C145733&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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