Bicyclo[2.2.1]-2,5-heptadiene-2,3-dicarboxylic acid

Other names: Bicyclo(2.2.1)hepta-2,5-diene-2,3-dicarboxylic acid
2,5-Norbornadiene-2,3-dicarboxylic acid
Inchi: InChI=1S/C9H8O4/c10-8(11)6-4-1-2-5(3-4)7(6)9(12)13/h1-2,4-5H,3H2,(H,10,11)(H,12,13
InchiKey: NRIMHVFWRMABGJ-UHFFFAOYSA-N
Formula: C9H8O4
SMILES: O=C(O)C1=C(C(=O)O)C2C=CC1C2
Mol. weight [g/mol]: 180.16
CAS: 15872-28-3

Physical Properties

Property code	Value	Unit	Source
gf	-356.52	kJ/mol	Joback Method
hf	-526.65	kJ/mol	Joback Method
hfus	26.28	kJ/mol	Joback Method
hvap	84.38	kJ/mol	Joback Method
log10ws	-0.80		Crippen Method
logp	0.658		Crippen Method
mcvol	122.230	ml/mol	McGowan Method
pc	4789.21	kPa	Joback Method
tb	723.45	K	Joback Method
tc	921.83	K	Joback Method
tf	471.61	K	Joback Method
vc	0.468	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	339.14	J/mol×K	723.45	Joback Method
cpg	373.01	J/mol×K	888.76	Joback Method
cpg	366.98	J/mol×K	855.70	Joback Method
cpg	360.62	J/mol×K	822.64	Joback Method
cpg	353.90	J/mol×K	789.58	Joback Method
cpg	346.75	J/mol×K	756.51	Joback Method
cpg	378.78	J/mol×K	921.83	Joback Method

dvisc	0.0001010	Pa×s	723.45	Joback Method
dvisc	0.0001416	Pa×s	681.48	Joback Method
dvisc	0.0002078	Pa×s	639.50	Joback Method
dvisc	0.0003216	Pa×s	597.53	Joback Method
dvisc	0.0005317	Pa×s	555.56	Joback Method
dvisc	0.0009545	Pa×s	513.58	Joback Method
dvisc	0.0019014	Pa×s	471.61	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=C15872283&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