7, 7-Dimethoxy-1, 4, 5, 6-tetrachlorobicyclo [2. 2. 1]-5-heptene-2-carboxylic acid

Inchi: InChI=1S/C10H10Cl4O4/c1-17-10(18-2)8(13)3-4(7(15)16)9(10,14)6(12)5(8)11/h4H,3H2,

InchiKey: QWEKUMJAPFNRMO-UHFFFAOYSA-N

Formula: C10H10Cl4O4

SMILES: COC1(OC)C2(Cl)CC(C(=O)O)C1(Cl)C(Cl)=C2Cl

Mol. weight [g/mol]: 336.00

CAS: 124715-79-3

Physical Properties

Property code	Value	Unit	Source
gf	-401.93	kJ/mol	Joback Method
hf	-662.62	kJ/mol	Joback Method
hfus	24.37	kJ/mol	Joback Method
hvap	81.18	kJ/mol	Joback Method
log10ws	-3.12		Crippen Method
logp	2.738		Crippen Method
mcvol	193.880	ml/mol	McGowan Method
pc	2937.70	kPa	Joback Method
tb	787.06	K	Joback Method
tc	1014.89	K	Joback Method
tf	598.73	K	Joback Method
vc	0.737	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	487.47	J/mol×K	787.06	Joback Method
cpg	499.42	J/mol×K	825.03	Joback Method
cpg	512.35	J/mol×K	863.00	Joback Method
cpg	526.58	J/mol×K	900.97	Joback Method
cpg	542.44	J/mol×K	938.94	Joback Method
cpg	560.26	J/mol×K	976.91	Joback Method
cpg	580.36	J/mol×K	1014.89	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C124715793&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
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