Tetramethyl bicyclo[2.2.2]-7-octene-2,3,5,6-tetracarboxylate

Inchi: InChI=1S/C16H20O8/c1-21-13(17)9-7-5-6-8(10(9)14(18)22-2)12(16(20)24-4)11(7)15(19)23-3

InchiKey: CAOGMEMPDFAZPR-UHFFFAOYSA-N

Formula: C16H20O8

SMILES: COC(=O)C1C2C=CC(C1C(=O)OC)C(C(=O)OC)C2C(=O)OC

Mol. weight [g/mol]: 340.33

CAS: 72598-54-0

Physical Properties

Property code	Value	Unit	Source
gf	-755.42	kJ/mol	Joback Method
hf	-1243.07	kJ/mol	Joback Method
hfus	45.92	kJ/mol	Joback Method
hvap	87.06	kJ/mol	Joback Method
log10ws	-0.16		Crippen Method
logp	-0.041		Crippen Method
mcvol	240.040	ml/mol	McGowan Method
pc	1801.56	kPa	Joback Method
tb	873.14	K	Joback Method
tc	1087.28	K	Joback Method
tf	571.36	K	Joback Method
vc	0.907	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	791.07	J/mol×K	873.14	Joback Method
cpg	804.78	J/mol×K	908.83	Joback Method
cpg	817.05	J/mol×K	944.52	Joback Method
cpg	827.87	J/mol×K	980.21	Joback Method
cpg	837.21	J/mol×K	1015.90	Joback Method
cpg	845.08	J/mol×K	1051.59	Joback Method
cpg	851.45	J/mol×K	1087.28	Joback Method
dvisc	0.0018509	Pa×s	571.36	Joback Method
dvisc	0.0014759	Pa×s	621.66	Joback Method

dvisc	0.0012175	Pa×s	671.95	Joback Method
dvisc	0.0010316	Pa×s	722.25	Joback Method
dvisc	0.0008932	Pa×s	772.55	Joback Method
dvisc	0.0007870	Pa×s	822.84	Joback Method
dvisc	0.0007037	Pa×s	873.14	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=C72598540&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

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