Trans-1,3-cyclobutanediol, 2,2,4,4-tetramethyl-, diacetate

Inchi: InChI=1S/C12H20O4/c1-7(13)15-9-11(3,4)10(12(9,5)6)16-8(2)14/h9-10H,1-6H3
InchiKey: INCLPCMHSAPRGR-UHFFFAOYSA-N
Formula: C12H20O4
SMILES: CC(=O)OC1C(C)(C)C(OC(C)=O)C1(C)C
Mol. weight [g/mol]: 228.28
CAS: 4868-08-0

Physical Properties

Property code	Value	Unit	Source
gf	-403.14	kJ/mol	Joback Method
hf	-744.51	kJ/mol	Joback Method
hfus	19.06	kJ/mol	Joback Method
hvap	57.47	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	1.916		Crippen Method
mcvol	183.960	ml/mol	McGowan Method
pc	2200.01	kPa	Joback Method
tb	624.02	K	Joback Method
tc	830.34	K	Joback Method
tf	418.82	K	Joback Method
vc	0.698	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.46	J/mol×K	624.02	Joback Method
cpg	519.92	J/mol×K	658.41	Joback Method
cpg	535.70	J/mol×K	692.79	Joback Method
cpg	550.95	J/mol×K	727.18	Joback Method
cpg	565.80	J/mol×K	761.56	Joback Method
cpg	580.40	J/mol×K	795.95	Joback Method
cpg	594.89	J/mol×K	830.34	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4868080&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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