Bis(3-oxobutan-2-yl) phthalate

Other names: 1,2-Benzenedicarboxylic acid, bis(3-oxobutan-2-yl) ester
Bis(3-oxobutan-2-yl)-1,2-benzenedicarboxylate
Inchi: InChI=1S/C16H18O6/c1-9(17)11(3)21-15(19)13-7-5-6-8-14(13)16(20)22-12(4)10(2)18/h5
InchiKey: SPKUAVROPJEOQR-UHFFFAOYSA-N
Formula: C16H18O6
SMILES: CC(=O)C(C)OC(=O)c1ccccc1C(=O)OC(C)C(C)=O
Mol. weight [g/mol]: 306.31

Physical Properties

Property code	Value	Unit	Source
gf	-543.94	kJ/mol	Joback Method
hf	-873.83	kJ/mol	Joback Method
hfus	32.57	kJ/mol	Joback Method
hvap	85.18	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	1.955		Crippen Method
mcvol	230.560	ml/mol	McGowan Method
pc	2058.62	kPa	Joback Method
rinpol	2101.00		NIST Webbook
rinpol	2101.00		NIST Webbook
tb	856.58	K	Joback Method
tc	1076.91	K	Joback Method
tf	523.20	K	Joback Method
vc	0.872	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	677.45	J/mol×K	856.58	Joback Method
cpg	689.35	J/mol×K	893.30	Joback Method
cpg	700.09	J/mol×K	930.02	Joback Method
cpg	709.68	J/mol×K	966.75	Joback Method
cpg	718.12	J/mol×K	1003.47	Joback Method
cpg	725.42	J/mol×K	1040.19	Joback Method

cpg	731.60	J/mol×K	1076.91	Joback Method
dvisc	0.0007442	Pa×s	523.20	Joback Method
dvisc	0.0004211	Pa×s	578.76	Joback Method
dvisc	0.0002632	Pa×s	634.33	Joback Method
dvisc	0.0001775	Pa×s	689.89	Joback Method
dvisc	0.0001269	Pa×s	745.45	Joback Method
dvisc	0.0000951	Pa×s	801.02	Joback Method
dvisc	0.0000740	Pa×s	856.58	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U373499&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
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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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