Propanedioic acid, (phenylmethylene)-

Other names:	Malonic acid, benzylidene- Benzylidenemalonic acid
Inchi:	InChI=1S/C10H8O4/c11-9(12)8(10(13)14)6-7-4-2-1-3-5-7/h1-6H,(H,11,12)(H,13,14)
InchiKey:	KXTAOXNYQGASTA-UHFFFAOYSA-N
Formula:	C10H8O4
SMILES:	O=C(O)C(=Cc1ccccc1)C(=O)O
Mol. weight [g/mol]:	192.17
CAS:	584-45-2

Physical Properties

Property code	Value	Unit	Source
chs	-4363.10	kJ/mol	NIST Webbook
gf	-314.08	kJ/mol	Joback Method
hf	-435.39	kJ/mol	Joback Method
hfs	-715.00	kJ/mol	NIST Webbook
hfus	25.96	kJ/mol	Joback Method
hvap	87.02	kJ/mol	Joback Method
log10ws	-1.33		Crippen Method
logp	1.239		Crippen Method
mcvol	138.580	ml/mol	McGowan Method
pc	4565.38	kPa	Joback Method
tb	751.02	K	Joback Method
tc	956.74	K	Joback Method
tf	431.34	K	Joback Method
vc	0.518	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	357.53	J/mol×K	751.02	Joback Method
cpg	364.98	J/mol×K	785.31	Joback Method
cpg	371.89	J/mol×K	819.59	Joback Method
cpg	378.31	J/mol×K	853.88	Joback Method
cpg	384.29	J/mol×K	888.17	Joback Method

cpg	389.87	J/mol×K	922.45	Joback Method
cpg	395.09	J/mol×K	956.74	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=C584452&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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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