Benzylmalonic acid

Other names:	Propanedioic acid, (phenylmethyl)-
	Malonic acid, benzyl-
	Malonic acid, 2-benzyl-
	USAF XR-36
	1,1-Ethanedicarboxylic acid, 2-phenyl-
	2-Benzylmalonic acid
	NSC 8068
Inchi:	InChI=1S/C10H10O4/c11-9(12)8(10(13)14)6-7-4-2-1-3-5-7/h1-5,8H,6H2,(H,11,12)(H,13,1
InchiKey:	JAEJSNFTJMYIEF-UHFFFAOYSA-N
Formula:	C10H10O4
SMILES:	O=C(O)C(Cc1ccccc1)C(=O)O
Mol. weight [g/mol]:	194.18
CAS:	616-75-1

Physical Properties

Property code	Value	Unit	Source
gf	-388.19	kJ/mol	Joback Method
hf	-548.10	kJ/mol	Joback Method
hfus	23.55	kJ/mol	Joback Method
hvap	86.59	kJ/mol	Joback Method
log10ws	-1.07		Crippen Method
logp	1.014		Crippen Method
mcvol	142.880	ml/mol	McGowan Method
pc	4277.45	kPa	Joback Method
tb	746.54	K	Joback Method
tc	946.57	K	Joback Method
tf	435.38	K	Joback Method
vc	0.531	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.78	J/mol×K	746.54	Joback Method
cpg	391.95	J/mol×K	779.88	Joback Method

cpg	399.54	J/mol×K	813.22	Joback Method
cpg	406.58	J/mol×K	846.55	Joback Method
cpg	413.09	J/mol×K	879.89	Joback Method
cpg	419.10	J/mol×K	913.23	Joback Method
cpg	424.64	J/mol×K	946.57	Joback Method
dvisc	0.0018592	Pa×s	435.38	Joback Method
dvisc	0.0005145	Pa×s	487.24	Joback Method
dvisc	0.0001823	Pa×s	539.10	Joback Method
dvisc	0.0000775	Pa×s	590.96	Joback Method
dvisc	0.0000378	Pa×s	642.82	Joback Method
dvisc	0.0000205	Pa×s	694.68	Joback Method
dvisc	0.0000121	Pa×s	746.54	Joback Method

Sources

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=C616751&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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