Benzylidenemalonaldehyde

Other names: Benzalmalonic dialdehyde
Inchi: InChI=1S/C10H8O2/c11-7-10(8-12)6-9-4-2-1-3-5-9/h1-8H
InchiKey: XMXUYXIFVYQLKJ-UHFFFAOYSA-N
Formula: C10H8O2
SMILES: O=CC(C=O)=Cc1ccccc1
Mol. weight [g/mol]: 160.17
CAS: 82700-43-4

Physical Properties

Property code	Value	Unit	Source
gf	18.36	kJ/mol	Joback Method
hf	-76.93	kJ/mol	Joback Method
hfus	19.17	kJ/mol	Joback Method
hvap	53.61	kJ/mol	Joback Method
log10ws	-1.69		Crippen Method
logp	1.468		Crippen Method
mcvol	126.840	ml/mol	McGowan Method
pc	3708.97	kPa	Joback Method
rinpol	1219.00		NIST Webbook
rinpol	1215.00		NIST Webbook
rinpol	1215.00		NIST Webbook
tb	556.24	K	Joback Method
tc	783.43	K	Joback Method
tf	293.84	K	Joback Method
vc	0.502	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.95	J/mol×K	556.24	Joback Method
cpg	287.44	J/mol×K	594.10	Joback Method
cpg	298.06	J/mol×K	631.97	Joback Method
cpg	307.86	J/mol×K	669.83	Joback Method
cpg	316.90	J/mol×K	707.70	Joback Method

cpg	325.24	J/mol×K	745.56	Joback Method
cpg	332.93	J/mol×K	783.43	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C82700434&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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume