

Dibenzyl malonate

Other names:	Propanedioic acid, bis(phenylmethyl) ester
Inchi:	InChI=1S/C17H16O4/c18-16(20-12-14-7-3-1-4-8-14)11-17(19)21-13-15-9-5-2-6-10-15/h1
InchiKey:	RYFCSKVXWRJEOB-UHFFFAOYSA-N
Formula:	C17H16O4
SMILES:	O=C(CC(=O)OCc1ccccc1)OCc1ccccc1
Mol. weight [g/mol]:	284.31
CAS:	15014-25-2

Physical Properties

Property code	Value	Unit	Source
gf	-150.76	kJ/mol	Joback Method
hf	-410.75	kJ/mol	Joback Method
hfus	33.44	kJ/mol	Joback Method
hvap	76.30	kJ/mol	Joback Method
log10ws	-3.86		Crippen Method
logp	2.863		Crippen Method
mcvol	217.750	ml/mol	McGowan Method
pc	2276.24	kPa	Joback Method
tb	794.30	K	Joback Method
tc	1025.52	K	Joback Method
tf	478.51	K	Joback Method
vc	0.820	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	614.11	J/mol×K	794.30	Joback Method
cpg	628.00	J/mol×K	832.84	Joback Method
cpg	640.64	J/mol×K	871.37	Joback Method
cpg	652.08	J/mol×K	909.91	Joback Method
cpg	662.36	J/mol×K	948.45	Joback Method
cpg	671.52	J/mol×K	986.98	Joback Method
cpg	679.59	J/mol×K	1025.52	Joback Method
dvisc	0.0007896	Pa×s	478.51	Joback Method

dvisc	0.0004501	Pa×s	531.14	Joback Method
dvisc	0.0002839	Pa×s	583.77	Joback Method
dvisc	0.0001933	Pa×s	636.40	Joback Method
dvisc	0.0001395	Pa×s	689.04	Joback Method
dvisc	0.0001055	Pa×s	741.67	Joback Method
dvisc	0.0000828	Pa×s	794.30	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	461.20	K	0.03	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15014252&Units=SI

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature

tf: Normal melting (fusion) point
vc: Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/34-521-5/Dibenzyl-malonate.pdf>

Generated by Cheméo on 2025-12-06 00:49:12.880418556 +0000 UTC m=+4730350.410459220.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.