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

Physical Properties

Property code	Value	Unit	Source
hf	-494.38	kJ/mol	Cheméo Relay (1.0)
hfus	33.44	kJ/mol	Joback Method
hvap	105.69	kJ/mol	Cheméo Relay (1.0)
ie	8.66	eV	Cheméo Relay (1.0)
log10ws	-3.64		Cheméo Relay (1.0)
logp	2.863		Crippen Method
mcvol	217.750	ml/mol	McGowan Method
pc	2276.24	kPa	Joback Method
tb	625.54	K	Cheméo Relay (1.0)
tf	284.33	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	614.11	J/mol×K	794.30	Joback Method
cpg	679.59	J/mol×K	1025.52	Joback Method
cpg	671.52	J/mol×K	986.98	Joback Method
cpg	662.36	J/mol×K	948.45	Joback Method
cpg	652.08	J/mol×K	909.91	Joback Method
cpg	640.64	J/mol×K	871.37	Joback Method
cpg	628.00	J/mol×K	832.84	Joback Method
dvisc	0.0001933	Pa×s	636.40	Joback Method
dvisc	0.0000828	Pa×s	794.30	Joback Method
dvisc	0.0001055	Pa×s	741.67	Joback Method
dvisc	0.0001395	Pa×s	689.04	Joback Method

dvisc	0.0007896	Pa×s	478.51	Joback Method
dvisc	0.0002839	Pa×s	583.77	Joback Method
dvisc	0.0004501	Pa×s	531.14	Joback Method

Pressure Dependent Properties

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

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

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

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
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
tf: Normal melting (fusion) point