1,3-Propanedione, 2-bromo-1,3-diphenyl-

Other names:	Bromodibenzoylmethane
	Dibenzoylbromomethane
	Methane, dibenzoylbromo-
	2-Bromo-1,3-diphenyl-1,3-propanedione
Inchi:	InChI=1S/C15H11BrO2/c16-13(14(17)11-7-3-1-4-8-11)15(18)12-9-5-2-6-10-12/h1-10,13H
InchiKey:	BYAJHZYXPBREEK-UHFFFAOYSA-N
Formula:	C15H11BrO2
SMILES:	O=C(c1ccccc1)C(Br)C(=O)c1ccccc1
Mol. weight [g/mol]:	303.15
CAS:	728-84-7

Physical Properties

Property code	Value	Unit	Source
gf	54.28	kJ/mol	Joback Method
hf	-83.98	kJ/mol	Joback Method
hfus	27.65	kJ/mol	Joback Method
hvap	73.08	kJ/mol	Joback Method
log10ws	-4.57		Crippen Method
logp	3.516		Crippen Method
mcvol	195.330	ml/mol	McGowan Method
pc	3110.57	kPa	Joback Method
tb	769.42	K	Joback Method
tc	1031.47	K	Joback Method
tf	456.31	K	Joback Method
vc	0.728	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	490.00	J/mol×K	769.42	Joback Method
cpg	502.54	J/mol×K	813.10	Joback Method
cpg	513.85	J/mol×K	856.77	Joback Method
cpg	524.06	J/mol×K	900.45	Joback Method
cpg	533.27	J/mol×K	944.12	Joback Method

cpg	541.60	J/mol×K	987.80	Joback Method
cpg	549.18	J/mol×K	1031.47	Joback Method
dvisc	0.0014639	Pa×s	456.31	Joback Method
dvisc	0.0008149	Pa×s	508.50	Joback Method
dvisc	0.0005059	Pa×s	560.68	Joback Method
dvisc	0.0003406	Pa×s	612.87	Joback Method
dvisc	0.0002440	Pa×s	665.05	Joback Method
dvisc	0.0001835	Pa×s	717.23	Joback Method
dvisc	0.0001434	Pa×s	769.42	Joback Method

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=C728847&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
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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