1-phenyl-2,3-butanedione

Other names: 1-phenylbutane-2, 3-dione
Inchi: InChI=1S/C10H10O2/c1-8(11)10(12)7-9-5-3-2-4-6-9/h2-6H,7H2,1H3
InchiKey: WZLKRAJHCPNZAA-UHFFFAOYSA-N
Formula: C10H10O2
SMILES: CC(=O)C(=O)Cc1ccccc1
Mol. weight [g/mol]: 162.19

Physical Properties

Property code	Value	Unit	Source
gf	-112.11	kJ/mol	Joback Method
hf	-238.36	kJ/mol	Joback Method
hfus	18.89	kJ/mol	Joback Method
hvap	53.62	kJ/mol	Joback Method
log10ws	-1.67		Crippen Method
logp	1.387		Crippen Method
mcvol	131.140	ml/mol	McGowan Method
pc	3376.28	kPa	Joback Method
rinpol	1212.00		NIST Webbook
rinpol	1230.00		NIST Webbook
rinpol	1212.00		NIST Webbook
rinpol	1211.00		NIST Webbook
rinpol	1230.00		NIST Webbook
rinpol	1211.00		NIST Webbook
ripol	2003.00		NIST Webbook
ripol	2003.00		NIST Webbook
tb	562.62	K	Joback Method
tc	786.27	K	Joback Method
tf	328.74	K	Joback Method
vc	0.499	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	293.17	J/mol×K	562.62	Joback Method

cpg	305.78	J/mol×K	599.90	Joback Method
cpg	317.53	J/mol×K	637.17	Joback Method
cpg	328.47	J/mol×K	674.45	Joback Method
cpg	338.63	J/mol×K	711.72	Joback Method
cpg	348.04	J/mol×K	749.00	Joback Method
cpg	356.75	J/mol×K	786.27	Joback Method
dvisc	0.0026820	Pa×s	328.74	Joback Method
dvisc	0.0015118	Pa×s	367.72	Joback Method
dvisc	0.0009511	Pa×s	406.70	Joback Method
dvisc	0.0006489	Pa×s	445.68	Joback Method
dvisc	0.0004708	Pa×s	484.66	Joback Method
dvisc	0.0003583	Pa×s	523.64	Joback Method
dvisc	0.0002832	Pa×s	562.62	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R225260&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume