2-CHLORO-BENZALACETONE

Other names: (o-Chlorobenzylidene)acetone
2-Chloro-benzalacetone
3-Buten-2-one, 4-(o-chlorophenyl)-
4-(2-Chlorophenyl)-3-buten-2-one
4-(2-Chlorophenyl)-but-3-en-2-one
o-Chlorobenzalacetone
Inchi: InChI=1S/C10H9ClO/c1-8(12)6-7-9-4-2-3-5-10(9)11/h2-7H,1H3/b7-6+
InchiKey: FHDSETHROOWFCQ-VOTSOKGWSA-N
Formula: C10H9ClO
SMILES: CC(=O)/C=C/c1ccccc1Cl
Mol. weight [g/mol]: 180.63

Physical Properties

Property code	Value	Unit	Source
hf	-100.57	kJ/mol	Cheméo Relay (1.0)
hfus	21.31	kJ/mol	Joback Method
ie	8.80	eV	NIST Webbook
ie	8.80	eV	NIST Webbook
ie	8.80 ± 0.10	eV	NIST Webbook
log10ws	-2.90		Cheméo Relay (1.0)
logp	2.942		Crippen Method
mcvol	137.510	ml/mol	McGowan Method
tb	543.09	K	Cheméo Relay (1.0)
tf	324.45	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	283.35	J/mol×K	555.32	Joback Method
cpg	295.44	J/mol×K	593.84	Joback Method
cpg	306.65	J/mol×K	632.36	Joback Method
cpg	317.05	J/mol×K	670.88	Joback Method
cpg	326.69	J/mol×K	709.40	Joback Method
cpg	335.63	J/mol×K	747.92	Joback Method

cpg	343.91	J/mol×K	786.44	Joback Method
dvisc	0.0020142	Pa×s	316.17	Joback Method
dvisc	0.0011317	Pa×s	356.03	Joback Method
dvisc	0.0007142	Pa×s	395.89	Joback Method
dvisc	0.0004903	Pa×s	435.75	Joback Method
dvisc	0.0003585	Pa×s	475.60	Joback Method
dvisc	0.0002751	Pa×s	515.46	Joback Method
dvisc	0.0002193	Pa×s	555.32	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C20766374&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
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point