

Cyclobutyl phenyl ketone

Other names:	Benzoylcyclobutane Methanone, (cyclobutyl)(phenyl)-
Inchi:	InChI=1S/C11H12O/c12-11(10-7-4-8-10)9-5-2-1-3-6-9/h1-3,5-6,10H,4,7-8H2
InchiKey:	MVEBDOSCXOQNAR-UHFFFAOYSA-N
Formula:	C11H12O
SMILES:	O=C(c1cccc1)C1CCC1
Mol. weight [g/mol]:	160.21
CAS:	5407-98-7

Physical Properties

Property code	Value	Unit	Source
gf	73.88	kJ/mol	Joback Method
hf	-79.78	kJ/mol	Joback Method
hfus	15.92	kJ/mol	Joback Method
hvap	49.19	kJ/mol	Joback Method
log10ws	-3.04		Crippen Method
logp	2.669		Crippen Method
mvol	132.800	ml/mol	McGowan Method
pc	3360.64	kPa	Joback Method
tb	533.00	K	NIST Webbook
tb	533.20	K	NIST Webbook
tc	779.21	K	Joback Method
tf	304.50	K	Joback Method
vc	0.498	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.56	J/molxK	542.64	Joback Method
cpg	324.22	J/molxK	582.07	Joback Method
cpg	339.63	J/molxK	621.50	Joback Method
cpg	353.86	J/molxK	660.93	Joback Method
cpg	367.00	J/molxK	700.35	Joback Method
cpg	379.11	J/molxK	739.78	Joback Method

cpg	390.28	J/mol×K	779.21	Joback Method
dvisc	0.0028214	Paxs	304.50	Joback Method
dvisc	0.0017093	Paxs	344.19	Joback Method
dvisc	0.0011486	Paxs	383.88	Joback Method
dvisc	0.0008315	Paxs	423.57	Joback Method
dvisc	0.0006363	Paxs	463.26	Joback Method
dvisc	0.0005079	Paxs	502.95	Joback Method
dvisc	0.0004189	Paxs	542.64	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	389.20	K	0.90	NIST Webbook
tbrp	405.00 ± 1.00	K	2.00	NIST Webbook

Sources

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=C5407987&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
mvol:	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

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