

Cyclohexanone, 2,6-bis(phenylmethylene)-

Other names:	Cyclohexanone, 2,6-dibenzylidene- 2,6-Bis(benzylidene)cyclohexanone 2,6-Dibenzylidenecyclohexanone 2,6-dibenzylidenecyclohexan-1-one
Inchi:	InChI=1S/C20H18O/c21-20-18(14-16-8-3-1-4-9-16)12-7-13-19(20)15-17-10-5-2-6-11-17
InchiKey:	CTKKGXDAWIAYSA-JSAVKQRWSA-N
Formula:	C20H18O
SMILES:	O=C1C(=Cc2ccccc2)CCCC1=Cc1ccccc1
Mol. weight [g/mol]:	274.36
CAS:	897-78-9

Physical Properties

Property code	Value	Unit	Source
gf	342.83	kJ/mol	Joback Method
hf	105.95	kJ/mol	Joback Method
hfus	26.56	kJ/mol	Joback Method
hvap	71.23	kJ/mol	Joback Method
log10ws	-5.62		Crippen Method
logp	4.907		Crippen Method
mcvol	227.250	ml/mol	McGowan Method
pc	2173.43	kPa	Joback Method
tb	815.68	K	Joback Method
tc	1088.05	K	Joback Method
tf	468.56	K	Joback Method
vc	0.847	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	660.53	J/molxK	815.68	Joback Method
cpg	678.66	J/molxK	861.07	Joback Method
cpg	695.03	J/molxK	906.47	Joback Method
cpg	709.75	J/molxK	951.86	Joback Method
cpg	722.93	J/molxK	997.26	Joback Method

cpg	734.70	J/mol×K	1042.65	Joback Method
cpg	745.15	J/mol×K	1088.05	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C897789&Units=SI

Legend

cpg:	Ideal gas heat capacity
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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