Dibenzosuberone

Other names:	5H-Dibenzo[a,d]cyclohepten-5-one, 10,11-dihydro- Dibenzosuberan-5-one Dibenzo[a,d]cycloheptadien-5-one Dibenzo[a,d]cyclohepta[1,4]dien-5-one 10,11-Dihydrodibenzo[a,d]cyclohepten-5-one 2,3:6,7-Dibenzosuberone 10,11-Dihydro-5H-dibenzo(a,d)cyclohepten-5-one 5-Dibenzosuberone Dibenzocycloheptadienone Dibenzocycloheptenone NSC 49727 dibenzo(b,f)cycloheptan-1-one
Inchi:	InChI=1S/C15H12O/c16-15-13-7-3-1-5-11(13)9-10-12-6-2-4-8-14(12)15/h1-8H,9-10H2
InchiKey:	BMVWCPGVLSILMU-UHFFFAOYSA-N
Formula:	C15H12O
SMILES:	O=C1c2ccccc2CCc2ccccc21
Mol. weight [g/mol]:	208.26
CAS:	1210-35-1

Physical Properties

Property code	Value	Unit	Source
chs	-7496.00 ± 3.40	kJ/mol	NIST Webbook
gf	226.85	kJ/mol	Joback Method
hf	52.63	kJ/mol	Joback Method
hfs	-123.50 ± 3.40	kJ/mol	NIST Webbook
hfus	18.48	kJ/mol	Joback Method
hsub	109.30	kJ/mol	NIST Webbook
hvap	59.33	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	3.016		Crippen Method
mcvol	165.400	ml/mol	McGowan Method
pc	2992.59	kPa	Joback Method
tb	685.15	K	Joback Method
tc	951.73	K	Joback Method
tf	427.09	K	Joback Method
vc	0.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	501.30	J/mol×K	907.30	Joback Method
cpg	431.61	J/mol×K	685.15	Joback Method
cpg	448.13	J/mol×K	729.58	Joback Method
cpg	463.26	J/mol×K	774.01	Joback Method
cpg	477.10	J/mol×K	818.44	Joback Method
cpg	489.75	J/mol×K	862.87	Joback Method
cpg	511.84	J/mol×K	951.73	Joback Method
hfust	17.15	kJ/mol	305.50	NIST Webbook
hvapt	90.00 ± 1.50	kJ/mol	326.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	421.20	K	0.04	NIST Webbook

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=C1210351&Units=SI

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation

hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume