

1-Benzosuberone

Other names:	5H-Benzocyclohepten-5-one, 6,7,8,9-tetrahydro-Benzosuberone «alpha»-Benzosuberone Benzo(b)cycloheptan-1-one Benzosuberone 1-Benzosuberanone 2,3-Benzosuberone 5-Benzocycloheptanone 6,7,8,9-Tetrahydrobenzobicyclohepten-5-one 6,7,8,9-Tetrahydrobenzocyclohepten-5-one 6,7,8,9-Tetrahydro-5H-benzocyclohepten-5-one NSC 87961
Inchi:	InChI=1S/C11H12O/c12-11-8-4-2-6-9-5-1-3-7-10(9)11/h1,3,5,7H,2,4,6,8H2
InchiKey:	KWHUHTFXMNQHAA-UHFFFAOYSA-N
Formula:	C11H12O
SMILES:	O=C1CCCCc2ccccc21
Mol. weight [g/mol]:	160.21
CAS:	826-73-3

Physical Properties

Property code	Value	Unit	Source
gf	66.19	kJ/mol	Joback Method
hf	-102.19	kJ/mol	Joback Method
hfus	10.27	kJ/mol	Joback Method
hvap	47.83	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	2.596		Crippen Method
mcvol	132.800	ml/mol	McGowan Method
pc	3419.86	kPa	Joback Method
tb	543.20	K	NIST Webbook
tc	823.95	K	Joback Method
tf	336.03	K	Joback Method
vc	0.492	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	315.41	J/mol×K	570.51	Joback Method
cpg	332.90	J/mol×K	612.75	Joback Method
cpg	349.17	J/mol×K	654.99	Joback Method
cpg	364.27	J/mol×K	697.23	Joback Method
cpg	378.22	J/mol×K	739.47	Joback Method
cpg	391.07	J/mol×K	781.71	Joback Method
cpg	402.83	J/mol×K	823.95	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=C826733&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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