Tricyclo[3.3.1.1(3,7)]decane, 1-phenyl-

Other names: (Adamantyl-1)benzene
1-Phenyladamantane
Inchi: InChI=1S/C16H20/c1-2-4-15(5-3-1)16-9-12-6-13(10-16)8-14(7-12)11-16/h1-5,12-14H,6-1
InchiKey: XACJBFHSZJWBBP-UHFFFAOYSA-N
Formula: C16H20
SMILES: c1ccc(C23CC4CC(CC(C4)C2)C3)cc1
Mol. weight [g/mol]: 212.33
CAS: 780-68-7

Physical Properties

Property code	Value	Unit	Source
gf	353.20	kJ/mol	Joback Method
hf	70.10	kJ/mol	Joback Method
hfus	18.32	kJ/mol	Joback Method
hvap	51.94	kJ/mol	Joback Method
log10ws	-4.26		Crippen Method
logp	4.154		Crippen Method
mcvol	179.960	ml/mol	McGowan Method
pc	2510.03	kPa	Joback Method
tb	612.22	K	Joback Method
tc	861.95	K	Joback Method
tf	366.46	K	Joback Method
vc	0.683	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	505.19	J/mol×K	612.22	Joback Method
cpg	528.22	J/mol×K	653.84	Joback Method
cpg	549.47	J/mol×K	695.46	Joback Method
cpg	569.26	J/mol×K	737.09	Joback Method
cpg	587.92	J/mol×K	778.71	Joback Method
cpg	605.77	J/mol×K	820.33	Joback Method
cpg	623.12	J/mol×K	861.95	Joback Method

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=C780687&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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