(ADAMANTYL-1)BENZENE

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]: 212.34

Physical Properties

Property code	Value	Unit	Source
hf	-9.92	kJ/mol	Cheméo Relay (1.0)
hfus	18.32	kJ/mol	Joback Method
ie	8.46	eV	Cheméo Relay (1.0)
logp	4.154		Crippen Method
mcvol	179.960	ml/mol	McGowan Method
tf	465.82	K	Cheméo Relay (1.0)

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C780687&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point