4A-METHYL-4,4A,9,10-TETRAHYDRO-2(3H)-PHEN

Other names: 2(3H)-Phenanthrone, 4,4a,9,10-tetrahydro-4a-methyl-
4a-Methyl-4,4a,9,10-tetrahydro-2(3H)-phenanthrenone
4,4a,9,10-Tetrahydro-4a-methyl-2(3H)-phenanthrenone
Inchi: InChI=1S/C15H16O/c1-15-9-8-13(16)10-12(15)7-6-11-4-2-3-5-14(11)15/h2-5,10H,6-9H2
InchiKey: FSPGJSRKHCJARC-UHFFFAOYSA-N
Formula: C15H16O
SMILES: CC12CCC(=O)C=C1CCc1ccccc12
Mol. weight [g/mol]: 212.29

Physical Properties

Property code	Value	Unit	Source
hf	-13.07	kJ/mol	Cheméo Relay (1.0)
hfus	13.30	kJ/mol	Joback Method
hvap	84.31	kJ/mol	Cheméo Relay (1.0)
ie	8.57	eV	Cheméo Relay (1.0)
logp	3.180		Crippen Method
mcvol	174.000	ml/mol	McGowan Method
tb	601.21	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	475.96	J/mol×K	673.15	Joback Method
cpg	494.74	J/mol×K	716.88	Joback Method
cpg	512.40	J/mol×K	760.62	Joback Method
cpg	529.17	J/mol×K	804.35	Joback Method
cpg	545.33	J/mol×K	848.08	Joback Method
cpg	561.10	J/mol×K	891.82	Joback Method
cpg	576.75	J/mol×K	935.55	Joback Method

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6606344&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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):	

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature