Dibenzanthrone

Other names: Dibenzanthrone (violanthrone)
Inchi: InChI=1S/C34H16O2/c35-33-25-7-3-1-5-17(25)19-9-11-21-22-12-10-20-18-6-2-4-8-26(18
InchiKey: YKSGNOMLAIJTLT-UHFFFAOYSA-N
Formula: C34H16O2
SMILES: O=C1c2ccccc2-c2ccc3c4ccc5c6c(ccc(c7ccc1c2c73)c64)C(=O)c1ccccc1-5
Mol. weight [g/mol]: 456.50

Physical Properties

Property code	Value	Unit	Source
hf	288.31	kJ/mol	Cheméo Relay (1.0)
hfus	55.04	kJ/mol	Joback Method
ie	7.58	eV	Cheméo Relay (1.0)
log10ws	-11.93		Cheméo Relay (1.0)
logp	8.160		Crippen Method
mcvol	326.520	ml/mol	McGowan Method
tb	994.48	K	Cheméo Relay (1.0)
tf	649.57	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1171.86	J/mol×K	1311.78	Joback Method
cpg	1212.38	J/mol×K	1362.24	Joback Method
cpg	1257.73	J/mol×K	1412.69	Joback Method
cpg	1308.49	J/mol×K	1463.15	Joback Method
cpg	1365.28	J/mol×K	1513.61	Joback Method
cpg	1428.68	J/mol×K	1564.06	Joback Method
cpg	1499.29	J/mol×K	1614.52	Joback Method
hsubt	208.80	kJ/mol	530.50	NIST Webbook
hsubt	202.90	kJ/mol	542.00	NIST Webbook

Sources

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):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116712&Units=SI

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point