3',5'-Diisopropyl-4,4-dimethyl-3-phenyl-1,2-benzo

Inchi: InChI=1S/C22H28O/c1-14(2)16-12-18(15(3)4)20-19(13-16)21(5,6)22(20,23)17-10-8-7-9-
InchiKey: CTXNSPHJPSTTHQ-UHFFFAOYSA-N
Formula: C22H28O
SMILES: CC(C)c1cc(C(C)C)c2c(c1)C(C)(C)C2(O)c1ccccc1
Mol. weight [g/mol]: 308.46
CAS: 33574-16-2

Physical Properties

Property code	Value	Unit	Source
chs	-12440.60 ± 1.60	kJ/mol	NIST Webbook
gf	242.75	kJ/mol	Joback Method
hf	-101.00 ± 10.00	kJ/mol	NIST Webbook
hfs	-218.30 ± 3.30	kJ/mol	NIST Webbook
hfus	25.40	kJ/mol	Joback Method
hsub	117.00 ± 9.00	kJ/mol	NIST Webbook
hsub	117.30	kJ/mol	NIST Webbook
hsub	117.90	kJ/mol	NIST Webbook
hvap	84.14	kJ/mol	Joback Method
log10ws	-6.16		Crippen Method
logp	5.460		Crippen Method
mcvol	268.330	ml/mol	McGowan Method
pc	1675.53	kPa	Joback Method
tb	860.64	K	Joback Method
tc	1085.05	K	Joback Method
tf	523.94	K	Joback Method
vc	1.018	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	846.40	J/mol×K	860.64	Joback Method
cpg	867.22	J/mol×K	898.04	Joback Method
cpg	888.50	J/mol×K	935.44	Joback Method
cpg	910.54	J/mol×K	972.84	Joback Method

cpg	933.62	J/mol×K	1010.24	Joback Method
cpg	958.05	J/mol×K	1047.65	Joback Method
cpg	984.11	J/mol×K	1085.05	Joback Method

Sources

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=C33574162&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation 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