3-Methoxy-1,3,3-triphenylpropyne

Inchi: InChI=1S/C22H18O/c1-23-22(20-13-7-3-8-14-20,21-15-9-4-10-16-21)18-17-19-11-5-2-6-
InchiKey: RIAXKBQNFHZEPR-UHFFFAOYSA-N
Formula: C22H18O
SMILES: COC(C#Cc1ccccc1)(c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 298.38
CAS: 850-65-7

Physical Properties

Property code	Value	Unit	Source
chs	-11450.00	kJ/mol	NIST Webbook
gf	572.23	kJ/mol	Joback Method
hf	343.51	kJ/mol	Joback Method
hfs	205.00	kJ/mol	NIST Webbook
hfus	31.75	kJ/mol	Joback Method
hvap	74.66	kJ/mol	Joback Method
log10ws	-5.60		Crippen Method
logp	4.628		Crippen Method
mcvol	246.830	ml/mol	McGowan Method
pc	2113.89	kPa	Joback Method
tb	810.99	K	Joback Method
tc	1094.19	K	Joback Method
tf	547.71	K	Joback Method
vc	0.912	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	695.09	J/mol×K	810.99	Joback Method
cpg	713.20	J/mol×K	858.19	Joback Method
cpg	729.50	J/mol×K	905.39	Joback Method
cpg	744.22	J/mol×K	952.59	Joback Method
cpg	757.54	J/mol×K	999.79	Joback Method
cpg	769.68	J/mol×K	1046.99	Joback Method
cpg	780.84	J/mol×K	1094.19	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=C850657&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
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