2,4,6-Cycloheptatriene-1-carboxylic acid, 1-phenyl-, methyl ester

Inchi: InChI=1S/C15H14O2/c1-17-14(16)15(11-7-2-3-8-12-15)13-9-5-4-6-10-13/h2-12H,1H3

InchiKey: FUHBRHWSRVQTRY-UHFFFAOYSA-N

Formula: C15H14O2

SMILES: COC(=O)C1(c2ccccc2)C=CC=CC=C1

Mol. weight [g/mol]: 226.27

CAS: 32777-12-1

Physical Properties

Property code	Value	Unit	Source
gf	50.65	kJ/mol	Joback Method
hf	-124.46	kJ/mol	Joback Method
hfus	18.54	kJ/mol	Joback Method
hvap	60.74	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	2.780		Crippen Method
mcvol	182.130	ml/mol	McGowan Method
pc	2775.92	kPa	Joback Method
tb	667.11	K	Joback Method
tc	921.62	K	Joback Method
tf	387.43	K	Joback Method
vc	0.672	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	468.55	J/mol×K	667.11	Joback Method
cpg	485.85	J/mol×K	709.53	Joback Method
cpg	501.97	J/mol×K	751.95	Joback Method
cpg	517.09	J/mol×K	794.37	Joback Method
cpg	531.41	J/mol×K	836.79	Joback Method
cpg	545.11	J/mol×K	879.20	Joback Method
cpg	558.39	J/mol×K	921.62	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=C32777121&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	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