Ethyl 7-phenylnoracadiene-7-carboxylate

Inchi: InChI=1S/C16H16O2/c1-2-18-15(17)16(12-8-4-3-5-9-12)13-10-6-7-11-14(13)16/h3-11,13
InchiKey: SZHMIFJETAFZRP-UHFFFAOYSA-N
Formula: C16H16O2
SMILES: CCOC(=O)C1(c2ccccc2)C2C=CC=CC21
Mol. weight [g/mol]: 240.30
CAS: 339-98-0

Physical Properties

Property code	Value	Unit	Source
gf	118.45	kJ/mol	Joback Method
hf	-131.94	kJ/mol	Joback Method
hfus	25.41	kJ/mol	Joback Method
hvap	61.76	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method
logp	2.860		Crippen Method
mcvol	189.660	ml/mol	McGowan Method
pc	2480.12	kPa	Joback Method
tb	680.09	K	Joback Method
tc	919.63	K	Joback Method
tf	422.20	K	Joback Method
vc	0.723	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.59	J/mol×K	680.09	Joback Method
cpg	541.84	J/mol×K	720.01	Joback Method
cpg	558.06	J/mol×K	759.94	Joback Method
cpg	573.47	J/mol×K	799.86	Joback Method
cpg	588.29	J/mol×K	839.79	Joback Method
cpg	602.76	J/mol×K	879.71	Joback Method
cpg	617.08	J/mol×K	919.63	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C339980&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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