Methyl 7-(4-nitrophenyl)norcaradiene-7-carboxylate

Inchi: InChI=1S/C15H13NO4/c1-20-14(17)15(12-4-2-3-5-13(12)15)10-6-8-11(9-7-10)16(18)19/h

InchiKey: JHCAALNYMCSOLH-UHFFFAOYSA-N

Formula: C15H13NO4

SMILES: COC(=O)C1(c2ccc([N+](=O)[O-])cc2)C2C=CC=CC21

Mol. weight [g/mol]: 271.27

CAS: 32777-10-9

Physical Properties

Property code	Value	Unit	Source
gf	135.95	kJ/mol	Joback Method
hf	-133.53	kJ/mol	Joback Method
hfus	33.79	kJ/mol	Joback Method
hvap	76.79	kJ/mol	Joback Method
log10ws	-3.40		Crippen Method
logp	2.378		Crippen Method
mcvol	192.990	ml/mol	McGowan Method
pc	2726.86	kPa	Joback Method
tb	814.03	K	Joback Method
tc	1077.12	K	Joback Method
tf	567.06	K	Joback Method
vc	0.749	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	573.95	J/mol×K	814.03	Joback Method
cpg	589.22	J/mol×K	857.88	Joback Method
cpg	604.17	J/mol×K	901.73	Joback Method
cpg	619.09	J/mol×K	945.57	Joback Method
cpg	634.28	J/mol×K	989.42	Joback Method
cpg	650.02	J/mol×K	1033.27	Joback Method
cpg	666.61	J/mol×K	1077.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C32777109&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