

Methyl 7-phenylnorcaradiene-7-carboxylate

Inchi:	InChI=1S/C15H14O2/c1-17-14(16)15(11-7-3-2-4-8-11)12-9-5-6-10-13(12)15/h2-10,12-13
InchiKey:	ZVIBIYYBAMLLDF-UHFFFAOYSA-N
Formula:	C15H14O2
SMILES:	COC(=O)C1(c2ccccc2)C2C=CC=CC21
Mol. weight [g/mol]:	226.27
CAS:	32777-09-6

Physical Properties

Property code	Value	Unit	Source
gf	110.03	kJ/mol	Joback Method
hf	-111.30	kJ/mol	Joback Method
hfus	22.82	kJ/mol	Joback Method
hvap	59.54	kJ/mol	Joback Method
log10ws	-2.75		Crippen Method
logp	2.469		Crippen Method
mcvol	175.570	ml/mol	McGowan Method
pc	2735.42	kPa	Joback Method
tb	657.21	K	Joback Method
tc	901.95	K	Joback Method
tf	410.93	K	Joback Method
vc	0.666	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	472.74	J/molxK	657.21	Joback Method
cpg	489.53	J/molxK	698.00	Joback Method
cpg	505.20	J/molxK	738.79	Joback Method
cpg	520.00	J/molxK	779.58	Joback Method
cpg	534.16	J/molxK	820.37	Joback Method
cpg	547.91	J/molxK	861.16	Joback Method
cpg	561.49	J/molxK	901.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C32777096&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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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