Isoxadifen-ethyl

Other names: 3-Isoxazolecarboxylic acid, 4,5-dihydro-5,5-diphenyl-, ethyl ester
Inchi: InChI=1S/C18H17NO3/c1-2-21-17(20)16-13-18(22-19-16,14-9-5-3-6-10-14)15-11-7-4-8-1
InchiKey: MWKVXOJATACCCH-UHFFFAOYSA-N
Formula: C18H17NO3
SMILES: CCOC(=O)C1=NOC(c2ccccc2)(c2ccccc2)C1
Mol. weight [g/mol]: 295.33
CAS: 163520-33-0

Physical Properties

Property code	Value	Unit	Source
gf	173.63	kJ/mol	Joback Method
hf	-125.59	kJ/mol	Joback Method
hfus	34.83	kJ/mol	Joback Method
hvap	80.15	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	3.270		Crippen Method
mcvol	225.090	ml/mol	McGowan Method
pc	2500.00	kPa	Joback Method
rinpol	2328.00		NIST Webbook
rinpol	2328.00		NIST Webbook
tb	841.20	K	Joback Method
tc	1106.12	K	Joback Method
tf	563.81	K	Joback Method
vc	0.847	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	688.77	J/mol×K	841.20	Joback Method
cpg	706.43	J/mol×K	885.35	Joback Method
cpg	723.24	J/mol×K	929.51	Joback Method
cpg	739.43	J/mol×K	973.66	Joback Method
cpg	755.22	J/mol×K	1017.81	Joback Method
cpg	770.84	J/mol×K	1061.97	Joback Method

cpg	786.51	J/mol×K	1106.12	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C163520330&Units=SI

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume