Cyclopropanecarboxylic acid, trans-2-phenyl-, 4-nitrophenyl ester

Inchi: InChI=1S/C16H13NO4/c18-16(15-10-14(15)11-4-2-1-3-5-11)21-13-8-6-12(7-9-13)17(19)
InchiKey: IRYHDWJCCUVCKC-UHFFFAOYSA-N
Formula: C16H13NO4
SMILES: O=C(Oc1ccc([N+](=O)[O-])cc1)C1CC1c1ccccc1
Mol. weight [g/mol]: 283.28

Physical Properties

Property code	Value	Unit	Source
gf	153.70	kJ/mol	Joback Method
hf	-115.08	kJ/mol	Joback Method
hfus	38.24	kJ/mol	Joback Method
hvap	81.77	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	3.304		Crippen Method
mcvol	202.780	ml/mol	McGowan Method
pc	2624.46	kPa	Joback Method
rinpol	2521.00		NIST Webbook
rinpol	2521.00		NIST Webbook
tb	854.02	K	Joback Method
tc	1119.93	K	Joback Method
tf	564.91	K	Joback Method
vc	0.777	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	605.73	J/mol×K	854.02	Joback Method
cpg	619.03	J/mol×K	898.34	Joback Method
cpg	631.03	J/mol×K	942.66	Joback Method
cpg	641.86	J/mol×K	986.98	Joback Method
cpg	651.64	J/mol×K	1031.29	Joback Method
cpg	660.49	J/mol×K	1075.61	Joback Method
cpg	668.54	J/mol×K	1119.93	Joback Method

Sources

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=U406884&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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