Ethaneperoxoic acid, 1-cyano-1-(2-methylphenyl)ethyl ester

Inchi: InChI=1S/C12H13NO3/c1-9-6-4-5-7-11(9)12(3,8-13)16-15-10(2)14/h4-7H,1-3H3
InchiKey: FFROOMNADSGFIK-UHFFFAOYSA-N
Formula: C12H13NO3
SMILES: CC(=O)OOC(C)(C#N)c1ccccc1C
Mol. weight [g/mol]: 219.24
CAS: 58422-67-6

Physical Properties

Property code	Value	Unit	Source
gf	-49.96	kJ/mol	Joback Method
hf	-286.84	kJ/mol	Joback Method
hfus	18.55	kJ/mol	Joback Method
hvap	65.99	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	2.228		Crippen Method
mcvol	170.870	ml/mol	McGowan Method
pc	2424.27	kPa	Joback Method
tb	703.18	K	Joback Method
tc	932.78	K	Joback Method
tf	425.74	K	Joback Method
vc	0.656	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	447.95	J/mol×K	703.18	Joback Method
cpg	460.31	J/mol×K	741.45	Joback Method
cpg	471.74	J/mol×K	779.71	Joback Method
cpg	482.27	J/mol×K	817.98	Joback Method
cpg	491.92	J/mol×K	856.25	Joback Method
cpg	500.73	J/mol×K	894.51	Joback Method
cpg	508.71	J/mol×K	932.78	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=C58422676&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume