Trinexapac-ethyl

Other names: Ethyl 4-(cyclopropyl-hydroxy-methylene)-3,5-dioxo-cyclohexane-1-carboxylate
Inchi: InChI=1S/C13H16O5/c1-2-18-13(17)8-5-9(14)11(10(15)6-8)12(16)7-3-4-7/h7-8,16H,2-6H
InchiKey: RVKCCVTVZORVGD-QXMHVHEDSA-N
Formula: C13H16O5
SMILES: CCOC(=O)C1CC(=O)C(=C(O)C2CC2)C(=O)C1
Mol. weight [g/mol]: 252.26
CAS: 95266-40-3

Physical Properties

Property code	Value	Unit	Source
gf	-435.23	kJ/mol	Joback Method
hf	-790.72	kJ/mol	Joback Method
hfus	24.30	kJ/mol	Joback Method
hvap	80.07	kJ/mol	Joback Method
log10ws	-1.67		Crippen Method
logp	1.320		Crippen Method
mcvol	184.460	ml/mol	McGowan Method
pc	2802.44	kPa	Joback Method
rinpol	2027.00		NIST Webbook
tb	833.76	K	Joback Method
tc	1059.77	K	Joback Method
tf	527.41	K	Joback Method
vc	0.695	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	594.76	J/mol×K	833.76	Joback Method
cpg	608.26	J/mol×K	871.43	Joback Method
cpg	620.53	J/mol×K	909.10	Joback Method
cpg	631.56	J/mol×K	946.76	Joback Method
cpg	641.34	J/mol×K	984.43	Joback Method
cpg	649.87	J/mol×K	1022.10	Joback Method
cpg	657.14	J/mol×K	1059.77	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C95266403&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume