cis-«alpha»-Necrodyl acetate

Inchi: InChI=1S/C12H20O2/c1-8-6-11(7-14-10(3)13)12(4,5)9(8)2/h6,9,11H,7H2,1-5H3/t9-,11-/m
InchiKey: LZTCNNXHQNNINB-MWLCHTKSSA-N
Formula: C12H20O2
SMILES: CC(=O)OCC1C=C(C)C(C)C1(C)C
Mol. weight [g/mol]: 196.29

Physical Properties

Property code	Value	Unit	Source
gf	-147.79	kJ/mol	Joback Method
hf	-454.46	kJ/mol	Joback Method
hfus	20.23	kJ/mol	Joback Method
hvap	50.90	kJ/mol	Joback Method
log10ws	-2.73		Crippen Method
logp	2.788		Crippen Method
mcvol	172.220	ml/mol	McGowan Method
pc	2175.46	kPa	Joback Method
rinpol	1287.00		NIST Webbook
tb	560.57	K	Joback Method
tc	763.38	K	Joback Method
tf	336.76	K	Joback Method
vc	0.654	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	434.83	J/mol×K	560.57	Joback Method
cpg	452.31	J/mol×K	594.37	Joback Method
cpg	468.92	J/mol×K	628.17	Joback Method
cpg	484.73	J/mol×K	661.98	Joback Method
cpg	499.82	J/mol×K	695.78	Joback Method
cpg	514.26	J/mol×K	729.58	Joback Method
cpg	528.12	J/mol×K	763.38	Joback Method

Sources

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=R342246&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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