(E)-3,7-Dimethylocta-2,6-dienyl ethyl carbonate

Inchi: InChI=1S/C13H22O3/c1-5-15-13(14)16-10-9-12(4)8-6-7-11(2)3/h7,9H,5-6,8,10H2,1-4H3/
InchiKey: VHCQYGMNMOULRZ-FMIVXFBMSA-N
Formula: C13H22O3
SMILES: CCOC(=O)OCC=C(C)CCC=C(C)C
Mol. weight [g/mol]: 226.31

Physical Properties

Property code	Value	Unit	Source
gf	-137.00	kJ/mol	Joback Method
hf	-473.81	kJ/mol	Joback Method
hfus	31.18	kJ/mol	Joback Method
hvap	56.17	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	3.852		Crippen Method
mcvol	198.740	ml/mol	McGowan Method
pc	1853.11	kPa	Joback Method
rinpol	1553.00		NIST Webbook
rinpol	1553.00		NIST Webbook
tb	603.63	K	Joback Method
tc	790.05	K	Joback Method
tf	292.58	K	Joback Method
vc	0.767	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.39	J/mol×K	603.63	Joback Method
cpg	519.07	J/mol×K	634.70	Joback Method
cpg	534.02	J/mol×K	665.77	Joback Method
cpg	548.25	J/mol×K	696.84	Joback Method
cpg	561.79	J/mol×K	727.91	Joback Method
cpg	574.67	J/mol×K	758.98	Joback Method
cpg	586.90	J/mol×K	790.05	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=U373767&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