3,7-Dimethyloct-6-enyl ethyl carbonate

Inchi: InChI=1S/C13H24O3/c1-5-15-13(14)16-10-9-12(4)8-6-7-11(2)3/h7,12H,5-6,8-10H2,1-4H
InchiKey: GXKOFANEAPTOJI-UHFFFAOYSA-N
Formula: C13H24O3
SMILES: CCOC(=O)OCCC(C)CCC=C(C)C
Mol. weight [g/mol]: 228.33

Physical Properties

Property code	Value	Unit	Source
gf	-211.11	kJ/mol	Joback Method
hf	-586.52	kJ/mol	Joback Method
hfus	28.77	kJ/mol	Joback Method
hvap	55.75	kJ/mol	Joback Method
log10ws	-3.80		Crippen Method
logp	3.932		Crippen Method
mcvol	203.040	ml/mol	McGowan Method
pc	1777.34	kPa	Joback Method
rinpol	1514.00		NIST Webbook
tb	599.15	K	Joback Method
tc	779.29	K	Joback Method
tf	296.62	K	Joback Method
vc	0.780	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	523.94	J/mol×K	599.15	Joback Method
cpg	540.16	J/mol×K	629.17	Joback Method
cpg	555.66	J/mol×K	659.20	Joback Method
cpg	570.47	J/mol×K	689.22	Joback Method
cpg	584.60	J/mol×K	719.24	Joback Method
cpg	598.05	J/mol×K	749.26	Joback Method
cpg	610.84	J/mol×K	779.29	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373781&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

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