6,6-dimethoxy-2,5,5-trimethylhex-2-ene

Other names: Amarocite
Inchi: InChI=1S/C11H22O2/c1-9(2)7-8-11(3,4)10(12-5)13-6/h7,10H,8H2,1-6H3
InchiKey: RDHNTAXPFZIMDN-UHFFFAOYSA-N
Formula: C11H22O2
SMILES: COC(OC)C(C)(C)CC=C(C)C
Mol. weight [g/mol]: 186.29
CAS: 67674-46-8

Physical Properties

Property code	Value	Unit	Source
gf	-96.19	kJ/mol	Joback Method
hf	-441.41	kJ/mol	Joback Method
hfus	14.58	kJ/mol	Joback Method
hvap	43.25	kJ/mol	Joback Method
log10ws	-2.82		Crippen Method
logp	2.988		Crippen Method
mcvol	173.290	ml/mol	McGowan Method
pc	2021.76	kPa	Joback Method
rinpol	1166.60		NIST Webbook
rinpol	1166.60		NIST Webbook
tb	496.29	K	Joback Method
tc	681.55	K	Joback Method
tf	226.57	K	Joback Method
vc	0.651	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	401.76	J/mol×K	496.29	Joback Method
cpg	418.70	J/mol×K	527.17	Joback Method
cpg	434.87	J/mol×K	558.04	Joback Method
cpg	450.28	J/mol×K	588.92	Joback Method
cpg	464.96	J/mol×K	619.80	Joback Method
cpg	478.94	J/mol×K	650.67	Joback Method

cpg	492.23	J/mol×K	681.55	Joback Method

Sources

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=C67674468&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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