(Z)-8-decen-4,6-diyn-1-yl 3-methylbutanoate

Inchi: InChI=1S/C15H20O2/c1-4-5-6-7-8-9-10-11-12-17-15(16)13-14(2)3/h4-5,14H,10-13H2,1-3

InchiKey: KWRUHFXUFNAAJG-PLNGDYQASA-N

Formula: C15H20O2

SMILES: CC=CC#CC#CCCCOC(=O)CC(C)C

Mol. weight [g/mol]: 232.32

CAS: 126693-81-0

Physical Properties

Property code	Value	Unit	Source
gf	324.88	kJ/mol	Joback Method
hf	58.81	kJ/mol	Joback Method
hfus	40.32	kJ/mol	Joback Method
hvap	62.01	kJ/mol	Joback Method
log10ws	-4.17		Crippen Method
logp	2.939		Crippen Method
mcvol	208.150	ml/mol	McGowan Method
pc	2007.30	kPa	Joback Method
rinpol	1787.00		NIST Webbook
rinpol	1832.20		NIST Webbook
rinpol	1787.00		NIST Webbook
rinpol	1832.20		NIST Webbook
ripol	2480.00		NIST Webbook
ripol	2480.00		NIST Webbook
tb	640.61	K	Joback Method
tc	854.81	K	Joback Method
tf	523.09	K	Joback Method
vc	0.797	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	519.47	J/mol×K	640.61	Joback Method
cpg	535.91	J/mol×K	676.31	Joback Method
cpg	551.47	J/mol×K	712.01	Joback Method

cpg	566.18	J/mol×K	747.71	Joback Method
cpg	580.07	J/mol×K	783.41	Joback Method
cpg	593.17	J/mol×K	819.11	Joback Method
cpg	605.50	J/mol×K	854.81	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C126693810&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume