(E)-Deca-8-en-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-SNAWJCMRSA-N

Formula: C15H20O2

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

Mol. weight [g/mol]: 232.32

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	1878.30		NIST Webbook
rinpol	1878.30		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

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=U413671&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