(E,Z)-2,8-Decadien-4,6-diyn-1-yl 3-methylbutanoate

Inchi: InChI=1S/C15H18O2/c1-4-5-6-7-8-9-10-11-12-17-15(16)13-14(2)3/h4-5,10-11,14H,12-13

InchiKey: FPIBENZMUTVCEK-JWPKELMXSA-N

Formula: C15H18O2

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

Mol. weight [g/mol]: 230.30

CAS: 126665-85-8

Physical Properties

Property code	Value	Unit	Source
gf	405.10	kJ/mol	Joback Method
hf	176.03	kJ/mol	Joback Method
hfus	40.52	kJ/mol	Joback Method
hvap	61.97	kJ/mol	Joback Method
log10ws	-4.02		Crippen Method
logp	2.715		Crippen Method
mcvol	203.850	ml/mol	McGowan Method
pc	2104.20	kPa	Joback Method
rinpol	1888.80		NIST Webbook
rinpol	1851.00		NIST Webbook
rinpol	1851.00		NIST Webbook
rinpol	1888.80		NIST Webbook
ripol	2596.00		NIST Webbook
tb	644.77	K	Joback Method
tc	867.75	K	Joback Method
tf	518.01	K	Joback Method
vc	0.777	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	498.01	J/mol×K	644.77	Joback Method
cpg	513.94	J/mol×K	681.93	Joback Method
cpg	528.95	J/mol×K	719.10	Joback Method
cpg	543.10	J/mol×K	756.26	Joback Method

cpg	556.43	J/mol×K	793.42	Joback Method
cpg	568.99	J/mol×K	830.58	Joback Method
cpg	580.83	J/mol×K	867.75	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C126665858&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