(R)-5-Methyl-2-(prop-1-en-2-yl)hex-4-en-1-yl 2-methylbutanoate

Inchi: InChI=1S/C15H26O2/c1-7-13(6)15(16)17-10-14(12(4)5)9-8-11(2)3/h8,13-14H,4,7,9-10H2

InchiKey: WBUQEUATHWMFQO-UHFFFAOYSA-N

Formula: C15H26O2

SMILES: C=C(C)C(CC=C(C)C)COC(=O)C(C)CC

Mol. weight [g/mol]: 238.37

CAS: 17609-96-0

Physical Properties

Property code	Value	Unit	Source
gf	-12.42	kJ/mol	Joback Method
hf	-385.22	kJ/mol	Joback Method
hfus	26.65	kJ/mol	Joback Method
hvap	56.81	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	4.124		Crippen Method
mcvol	221.050	ml/mol	McGowan Method
pc	1610.29	kPa	Joback Method
rinpol	1512.60		NIST Webbook
tb	618.61	K	Joback Method
tc	805.10	K	Joback Method
tf	266.21	K	Joback Method
vc	0.851	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	578.77	J/mol×K	618.61	Joback Method
cpg	596.36	J/mol×K	649.69	Joback Method
cpg	613.08	J/mol×K	680.77	Joback Method
cpg	628.98	J/mol×K	711.86	Joback Method
cpg	644.07	J/mol×K	742.94	Joback Method
cpg	658.39	J/mol×K	774.02	Joback Method
cpg	671.96	J/mol×K	805.10	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=C17609960&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