

1,8(10)-p-Menthadien-9-yl 3-methylbutanoate

Inchi:	InChI=1S/C15H24O2/c1-11(2)9-15(16)17-10-13(4)14-7-5-12(3)6-8-14/h5,11,14H,4,6-10H
InchiKey:	YKJANZVKQMMPTB-UHFFFAOYSA-N
Formula:	C15H24O2
SMILES:	<chem>C=C(COC(=O)CC(C)C)C1CC=C(C)CC1</chem>
Mol. weight [g/mol]:	236.35

Physical Properties

Property code	Value	Unit	Source
gf	-36.87	kJ/mol	Joback Method
hf	-386.74	kJ/mol	Joback Method
hfus	23.95	kJ/mol	Joback Method
hvap	58.54	kJ/mol	Joback Method
log10ws	-4.08		Crippen Method
logp	3.878		Crippen Method
mcvol	210.190	ml/mol	McGowan Method
pc	1840.41	kPa	Joback Method
rinpol	1625.00		NIST Webbook
tb	638.70	K	Joback Method
tc	843.15	K	Joback Method
tf	320.91	K	Joback Method
vc	0.794	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	570.32	J/molxK	638.70	Joback Method
cpg	589.59	J/molxK	672.78	Joback Method
cpg	607.78	J/molxK	706.85	Joback Method
cpg	624.91	J/molxK	740.93	Joback Method
cpg	641.00	J/molxK	775.00	Joback Method
cpg	656.08	J/molxK	809.08	Joback Method
cpg	670.19	J/molxK	843.15	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=R589336&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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	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

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