1-p-Menthen-9-yl 3-methylbutanoate

Inchi: InChI=1S/C15H26O2/c1-11(2)9-15(16)17-10-13(4)14-7-5-12(3)6-8-14/h5,11,13-14H,6-10
InchiKey: VJJQDACGAQKNSG-UHFFFAOYSA-N
Formula: C15H26O2
SMILES: CC1=CCC(C(C)COC(=O)CC(C)C)CC1
Mol. weight [g/mol]: 238.37

Physical Properties

Property code	Value	Unit	Source
gf	-118.60	kJ/mol	Joback Method
hf	-507.66	kJ/mol	Joback Method
hfus	23.01	kJ/mol	Joback Method
hvap	58.75	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	3.958		Crippen Method
mcvol	214.490	ml/mol	McGowan Method
pc	1780.34	kPa	Joback Method
rinpol	1640.00		NIST Webbook
tb	641.70	K	Joback Method
tc	843.11	K	Joback Method
tf	321.63	K	Joback Method
vc	0.806	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	593.61	J/mol×K	641.70	Joback Method
cpg	613.50	J/mol×K	675.27	Joback Method
cpg	632.29	J/mol×K	708.84	Joback Method
cpg	650.01	J/mol×K	742.41	Joback Method
cpg	666.68	J/mol×K	775.97	Joback Method
cpg	682.31	J/mol×K	809.54	Joback Method
cpg	696.94	J/mol×K	843.11	Joback Method
dvisc	0.0035846	Pa×s	321.63	Joback Method
dvisc	0.0013886	Pa×s	374.98	Joback Method

dvisc	0.0006813	Pa×s	428.32	Joback Method
dvisc	0.0003913	Pa×s	481.67	Joback Method
dvisc	0.0002511	Pa×s	535.01	Joback Method
dvisc	0.0001746	Pa×s	588.36	Joback Method
dvisc	0.0001290	Pa×s	641.70	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R589425&Units=SI

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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