Terpinyl formate

Other names: «alpha»-Terpenyl formate
p-menth-1-en-8-yl formate
Inchi: InChI=1S/C11H18O2/c1-9-4-6-10(7-5-9)11(2,3)13-8-12/h4,8,10H,5-7H2,1-3H3
InchiKey: IPYLQIQMGUZFCK-UHFFFAOYSA-N
Formula: C11H18O2
SMILES: CC1=CCC(C(C)(C)OC=O)CC1
Mol. weight [g/mol]: 182.26
CAS: 2153-26-6

Physical Properties

Property code	Value	Unit	Source
gf	-115.16	kJ/mol	Joback Method
hf	-396.29	kJ/mol	Joback Method
hfus	12.98	kJ/mol	Joback Method
hvap	49.30	kJ/mol	Joback Method
log10ws	-2.91		Crippen Method
logp	2.684		Crippen Method
mcvol	158.130	ml/mol	McGowan Method
pc	2571.50	kPa	Joback Method
rinpol	1247.00		NIST Webbook
rinpol	1333.00		NIST Webbook
ripol	1666.00		NIST Webbook
ripol	1688.00		NIST Webbook
ripol	1688.00		NIST Webbook
ripol	1683.00		NIST Webbook
tb	542.62	K	Joback Method
tc	755.58	K	Joback Method
tf	301.04	K	Joback Method
vc	0.595	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	388.99	J/mol×K	542.62	Joback Method

cpg	468.19	J/mol×K	720.09	Joback Method
cpg	454.31	J/mol×K	684.60	Joback Method
cpg	439.49	J/mol×K	649.10	Joback Method
cpg	423.68	J/mol×K	613.61	Joback Method
cpg	406.86	J/mol×K	578.11	Joback Method
cpg	481.16	J/mol×K	755.58	Joback Method
dvisc	0.0002212	Pa×s	542.62	Joback Method
dvisc	0.0002920	Pa×s	502.36	Joback Method
dvisc	0.0004045	Pa×s	462.09	Joback Method
dvisc	0.0005963	Pa×s	421.83	Joback Method
dvisc	0.0009540	Pa×s	381.57	Joback Method
dvisc	0.0017053	Pa×s	341.30	Joback Method
dvisc	0.0035606	Pa×s	301.04	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=C2153266&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume