

Terpinyl valerate

Other names:	Terpenyl pentanoate «alpha»-Terpinyl n-pentanoate
Inchi:	InChI=1S/C15H26O2/c1-5-6-7-14(16)17-15(3,4)13-10-8-12(2)9-11-13/h8,13H,5-7,9-11H2
InchiKey:	GIHNOWFSKYCHNL-UHFFFAOYSA-N
Formula:	C15H26O2
SMILES:	CCCCC(=O)OC(C)(C)C1CC=C(C)CC1
Mol. weight [g/mol]:	238.37

Physical Properties

Property code	Value	Unit	Source
gf	-110.88	kJ/mol	Joback Method
hf	-505.85	kJ/mol	Joback Method
hfus	22.65	kJ/mol	Joback Method
hvap	58.23	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	4.245		Crippen Method
mcvol	214.490	ml/mol	McGowan Method
pc	1784.86	kPa	Joback Method
ripol	1921.00		NIST Webbook
tb	639.35	K	Joback Method
tc	843.85	K	Joback Method
tf	354.05	K	Joback Method
vc	0.807	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	595.39	J/molxK	639.35	Joback Method
cpg	615.35	J/molxK	673.43	Joback Method
cpg	634.14	J/molxK	707.52	Joback Method
cpg	651.80	J/molxK	741.60	Joback Method
cpg	668.36	J/molxK	775.68	Joback Method
cpg	683.87	J/molxK	809.77	Joback Method
cpg	698.37	J/molxK	843.85	Joback Method

dvisc	0.0023774	Paxs	354.05	Joback Method
dvisc	0.0010984	Paxs	401.60	Joback Method
dvisc	0.0005976	Paxs	449.15	Joback Method
dvisc	0.0003653	Paxs	496.70	Joback Method
dvisc	0.0002434	Paxs	544.25	Joback Method
dvisc	0.0001731	Paxs	591.80	Joback Method
dvisc	0.0001295	Paxs	639.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R181947&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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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