Isoeugenyl isovalerate

Inchi: InChI=1S/C15H20O3/c1-5-6-12-7-8-13(14(10-12)17-4)18-15(16)9-11(2)3/h5-8,10-11H,9H
InchiKey: JNVPTYXMIALTSY-AATRIKPKSA-N
Formula: C15H20O3
SMILES: CC=Cc1ccc(OC(=O)CC(C)C)c(OC)c1
Mol. weight [g/mol]: 248.32

Physical Properties

Property code	Value	Unit	Source
gf	-92.57	kJ/mol	Joback Method
hf	-404.42	kJ/mol	Joback Method
hfus	28.52	kJ/mol	Joback Method
hvap	63.72	kJ/mol	Joback Method
log10ws	-4.16		Crippen Method
logp	3.680		Crippen Method
mcvol	207.460	ml/mol	McGowan Method
pc	1944.08	kPa	Joback Method
rinpol	1814.00		NIST Webbook
tb	681.67	K	Joback Method
tc	890.17	K	Joback Method
tf	384.58	K	Joback Method
vc	0.783	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	551.65	J/mol×K	681.67	Joback Method
cpg	567.57	J/mol×K	716.42	Joback Method
cpg	582.57	J/mol×K	751.17	Joback Method
cpg	596.66	J/mol×K	785.92	Joback Method
cpg	609.86	J/mol×K	820.67	Joback Method
cpg	622.19	J/mol×K	855.42	Joback Method
cpg	633.67	J/mol×K	890.17	Joback Method
dvisc	0.0009687	Pa×s	384.58	Joback Method
dvisc	0.0005108	Pa×s	434.09	Joback Method

dvisc	0.0003070	Pa×s	483.61	Joback Method
dvisc	0.0002028	Pa×s	533.12	Joback Method
dvisc	0.0001438	Pa×s	582.64	Joback Method
dvisc	0.0001076	Pa×s	632.15	Joback Method
dvisc	0.0000840	Pa×s	681.67	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R224945&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume