5-methyl-2-(isopropyl)phenyl isovalerate

Other names: Thymyl isovalerate
Inchi: InChI=1S/C15H22O2/c1-10(2)8-15(16)17-14-9-12(5)6-7-13(14)11(3)4/h6-7,9-11H,8H2,1-
InchiKey: NZIACPHCVAFJBR-UHFFFAOYSA-N
Formula: C15H22O2
SMILES: Cc1ccc(C(C)C)c(OC(=O)CC(C)C)c1
Mol. weight [g/mol]: 234.33
CAS: 69844-33-3

Physical Properties

Property code	Value	Unit	Source
gf	-70.23	kJ/mol	Joback Method
hf	-394.70	kJ/mol	Joback Method
hfus	23.61	kJ/mol	Joback Method
hvap	60.96	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	4.070		Crippen Method
mcvol	205.890	ml/mol	McGowan Method
pc	1898.60	kPa	Joback Method
rinpol	1552.00		NIST Webbook
rinpol	1552.00		NIST Webbook
rinpol	1551.00		NIST Webbook
rinpol	1551.00		NIST Webbook
rinpol	1552.00		NIST Webbook
rinpol	1574.00		NIST Webbook
rinpol	1574.00		NIST Webbook
rinpol	1551.00		NIST Webbook
ripol	1975.00		NIST Webbook
ripol	1975.00		NIST Webbook
ripol	1975.00		NIST Webbook
tb	654.65	K	Joback Method
tc	861.20	K	Joback Method
tf	352.43	K	Joback Method
vc	0.779	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	546.69	J/mol×K	654.65	Joback Method
cpg	622.82	J/mol×K	826.77	Joback Method
cpg	609.43	J/mol×K	792.35	Joback Method
cpg	595.15	J/mol×K	757.92	Joback Method
cpg	579.94	J/mol×K	723.50	Joback Method
cpg	563.79	J/mol×K	689.07	Joback Method
cpg	635.32	J/mol×K	861.20	Joback Method
dvisc	0.0001154	Pa×s	654.65	Joback Method
dvisc	0.0001507	Pa×s	604.28	Joback Method
dvisc	0.0002067	Pa×s	553.91	Joback Method
dvisc	0.0003019	Pa×s	503.54	Joback Method
dvisc	0.0004797	Pa×s	453.17	Joback Method
dvisc	0.0008557	Pa×s	402.80	Joback Method
dvisc	0.0018013	Pa×s	352.43	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=C69844333&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