4-allyl-2-methoxyphenyl isovalerate

Other names: Eugenyl isovalerate
Inchi: InChI=1S/C15H20O3/c1-5-6-12-7-8-13(14(10-12)17-4)18-15(16)9-11(2)3/h5,7-8,10-11H,
InchiKey: PLUVLWUSXQCTNH-UHFFFAOYSA-N
Formula: C15H20O3
SMILES: C=CCc1ccc(OC(=O)CC(C)C)c(OC)c1
Mol. weight [g/mol]: 248.32
CAS: 61114-24-7

Physical Properties

Property code	Value	Unit	Source
gf	-84.95	kJ/mol	Joback Method
hf	-396.21	kJ/mol	Joback Method
hfus	27.04	kJ/mol	Joback Method
hvap	63.09	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	3.375		Crippen Method
mcvol	207.460	ml/mol	McGowan Method
pc	1927.05	kPa	Joback Method
rinpol	1864.10		NIST Webbook
rinpol	1864.10		NIST Webbook
tb	674.19	K	Joback Method
tc	878.75	K	Joback Method
tf	387.90	K	Joback Method
vc	0.784	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	550.80	J/mol×K	674.19	Joback Method
cpg	566.67	J/mol×K	708.28	Joback Method
cpg	581.63	J/mol×K	742.38	Joback Method
cpg	595.71	J/mol×K	776.47	Joback Method
cpg	608.90	J/mol×K	810.57	Joback Method
cpg	621.22	J/mol×K	844.66	Joback Method

cpg	632.69	J/mol×K	878.75	Joback Method
dvisc	0.0010372	Pa×s	387.90	Joback Method
dvisc	0.0005705	Pa×s	435.62	Joback Method
dvisc	0.0003531	Pa×s	483.33	Joback Method
dvisc	0.0002382	Pa×s	531.04	Joback Method
dvisc	0.0001715	Pa×s	578.76	Joback Method
dvisc	0.0001298	Pa×s	626.47	Joback Method
dvisc	0.0001022	Pa×s	674.19	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C61114247&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

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