5-Isopropyl-2-methylphenyl 3,5,5-trimethylhexanoate

Inchi: InChI=1S/C19H30O2/c1-13(2)16-9-8-15(4)17(11-16)21-18(20)10-14(3)12-19(5,6)7/h8-9,

InchiKey: RLEOHAZINPWGHO-UHFFFAOYSA-N

Formula: C19H30O2

SMILES: Cc1ccc(C(C)C)cc1OC(=O)CC(C)CC(C)(C)C

Mol. weight [g/mol]: 290.44

Physical Properties

Property code	Value	Unit	Source
gf	-33.71	kJ/mol	Joback Method
hf	-486.01	kJ/mol	Joback Method
hfus	26.56	kJ/mol	Joback Method
hvap	68.57	kJ/mol	Joback Method
log10ws	-5.89		Crippen Method
logp	5.486		Crippen Method
mcvol	262.250	ml/mol	McGowan Method
pc	1413.31	kPa	Joback Method
rinpol	1905.00		NIST Webbook
tb	742.94	K	Joback Method
tc	948.99	K	Joback Method
tf	399.93	K	Joback Method
vc	0.993	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	770.41	J/mol×K	742.94	Joback Method
cpg	789.22	J/mol×K	777.28	Joback Method
cpg	806.86	J/mol×K	811.62	Joback Method
cpg	823.38	J/mol×K	845.96	Joback Method
cpg	838.83	J/mol×K	880.30	Joback Method
cpg	853.26	J/mol×K	914.65	Joback Method
cpg	866.72	J/mol×K	948.99	Joback Method
dvisc	0.0013627	Pa×s	399.93	Joback Method
dvisc	0.0005830	Pa×s	457.10	Joback Method

dvisc	0.0003013	Pa×s	514.27	Joback Method
dvisc	0.0001777	Pa×s	571.44	Joback Method
dvisc	0.0001153	Pa×s	628.60	Joback Method
dvisc	0.0000805	Pa×s	685.77	Joback Method
dvisc	0.0000593	Pa×s	742.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378241&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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