

4-(1-Propenyl)-phenyl-2-methyl butyrate

Inchi:	InChI=1S/C14H18O2/c1-4-6-12-7-9-13(10-8-12)16-14(15)11(3)5-2/h4,6-11H,5H2,1-3H3/
InchiKey:	QVAWDXCSFUFEAT-GQCTYLIASA-N
Formula:	C14H18O2
SMILES:	CC=Cc1ccc(OC(=O)C(C)CC)cc1
Mol. weight [g/mol]:	218.29

Physical Properties

Property code	Value	Unit	Source
gf	13.64	kJ/mol	Joback Method
hf	-240.09	kJ/mol	Joback Method
hfus	25.13	kJ/mol	Joback Method
hvap	58.42	kJ/mol	Joback Method
log10ws	-4.04		Crippen Method
logp	3.671		Crippen Method
mcvol	187.500	ml/mol	McGowan Method
pc	2183.60	kPa	Joback Method
ripol	2284.00		NIST Webbook
ripol	2284.00		NIST Webbook
ripol	2284.00		NIST Webbook
tb	631.39	K	Joback Method
tc	844.45	K	Joback Method
tf	338.56	K	Joback Method
vc	0.710	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	473.31	J/molxK	631.39	Joback Method
cpg	489.29	J/molxK	666.90	Joback Method
cpg	504.31	J/molxK	702.41	Joback Method
cpg	518.41	J/molxK	737.92	Joback Method
cpg	531.62	J/molxK	773.43	Joback Method
cpg	543.99	J/molxK	808.94	Joback Method
cpg	555.54	J/molxK	844.45	Joback Method

dvisc	0.0018328	Paxs	338.56	Joback Method
dvisc	0.0008729	Paxs	387.37	Joback Method
dvisc	0.0004908	Paxs	436.17	Joback Method
dvisc	0.0003099	Paxs	484.98	Joback Method
dvisc	0.0002128	Paxs	533.78	Joback Method
dvisc	0.0001557	Paxs	582.59	Joback Method
dvisc	0.0001195	Paxs	631.39	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R418249&Units=SI

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
mvol:	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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