Pseudoisoeugenyl-2-methyl butyrate

Inchi: InChI=1S/C14H18O3/c1-5-6-11-7-8-12(13(9-11)16-4)17-14(15)10(2)3/h5-10H,1-4H3/b6-
InchiKey: HEOQGBRLGAJSLZ-AATRIKPKSA-N
Formula: C14H18O3
SMILES: CC=Cc1ccc(OC(=O)C(C)C)c(OC)c1
Mol. weight [g/mol]: 234.29

Physical Properties

Property code	Value	Unit	Source
gf	-100.99	kJ/mol	Joback Method
hf	-383.78	kJ/mol	Joback Method
hfus	25.93	kJ/mol	Joback Method
hvap	61.49	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	3.290		Crippen Method
mcvol	193.370	ml/mol	McGowan Method
pc	2119.73	kPa	Joback Method
rinpol	1792.00		NIST Webbook
rinpol	1795.00		NIST Webbook
rinpol	1792.00		NIST Webbook
ripol	2567.00		NIST Webbook
ripol	2567.00		NIST Webbook
tb	658.79	K	Joback Method
tc	870.40	K	Joback Method
tf	373.31	K	Joback Method
vc	0.728	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	499.19	J/mol×K	658.79	Joback Method
cpg	514.63	J/mol×K	694.06	Joback Method
cpg	529.19	J/mol×K	729.33	Joback Method
cpg	542.87	J/mol×K	764.60	Joback Method
cpg	555.70	J/mol×K	799.87	Joback Method

cpg	567.68	J/mol×K	835.13	Joback Method
cpg	578.83	J/mol×K	870.40	Joback Method
dvisc	0.0010266	Pa×s	373.31	Joback Method
dvisc	0.0005495	Pa×s	420.89	Joback Method
dvisc	0.0003339	Pa×s	468.47	Joback Method
dvisc	0.0002225	Pa×s	516.05	Joback Method
dvisc	0.0001587	Pa×s	563.63	Joback Method
dvisc	0.0001193	Pa×s	611.21	Joback Method
dvisc	0.0000935	Pa×s	658.79	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R240061&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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