Pseudoisoeugenyl 2-methylbutyrate II

Inchi: InChI=1S/C16H22O3/c1-5-8-12-9-10-14(15(11-12)18-4)19-16(17)13(6-2)7-3/h5,8-11,13H
InchiKey: KEANZVAQMYREAC-UHFFFAOYSA-N
Formula: C16H22O3
SMILES: CC=Cc1ccc(OC(=O)C(CC)CC)c(OC)c1
Mol. weight [g/mol]: 262.34

Physical Properties

Property code	Value	Unit	Source
gf	-84.15	kJ/mol	Joback Method
hf	-425.06	kJ/mol	Joback Method
hfus	31.11	kJ/mol	Joback Method
hvap	65.95	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	4.070		Crippen Method
mcvol	221.550	ml/mol	McGowan Method
pc	1789.39	kPa	Joback Method
rinpol	1792.00		NIST Webbook
rinpol	1792.00		NIST Webbook
tb	704.55	K	Joback Method
tc	910.32	K	Joback Method
tf	395.85	K	Joback Method
vc	0.840	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	605.42	J/mol×K	704.55	Joback Method
cpg	621.74	J/mol×K	738.85	Joback Method
cpg	637.10	J/mol×K	773.14	Joback Method
cpg	651.53	J/mol×K	807.44	Joback Method
cpg	665.05	J/mol×K	841.73	Joback Method
cpg	677.67	J/mol×K	876.03	Joback Method
cpg	689.42	J/mol×K	910.32	Joback Method
dvisc	0.0009069	Pa×s	395.85	Joback Method

dvisc	0.0004713	Pa×s	447.30	Joback Method
dvisc	0.0002804	Pa×s	498.75	Joback Method
dvisc	0.0001838	Pa×s	550.20	Joback Method
dvisc	0.0001295	Pa×s	601.65	Joback Method
dvisc	0.0000964	Pa×s	653.10	Joback Method
dvisc	0.0000750	Pa×s	704.55	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R510771&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