Benzoic acid, 2-(2-methoxyethyl)hexyl ester

Inchi: InChI=1S/C16H24O3/c1-3-4-8-14(11-12-18-2)13-19-16(17)15-9-6-5-7-10-15/h5-7,9-10,1
InchiKey: XPFIBKILBHEPLF-UHFFFAOYSA-N
Formula: C16H24O3
SMILES: CCCCC(CCOC)COC(=O)c1ccccc1
Mol. weight [g/mol]: 264.36

Physical Properties

Property code	Value	Unit	Source
gf	-145.11	kJ/mol	Joback Method
hf	-519.34	kJ/mol	Joback Method
hfus	31.69	kJ/mol	Joback Method
hvap	64.66	kJ/mol	Joback Method
log10ws	-3.91		Crippen Method
logp	3.686		Crippen Method
mcvol	225.850	ml/mol	McGowan Method
pc	1756.54	kPa	Joback Method
rinpol	1931.00		NIST Webbook
tb	690.43	K	Joback Method
tc	887.72	K	Joback Method
tf	375.89	K	Joback Method
vc	0.860	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	629.15	J/mol×K	690.43	Joback Method
cpg	646.23	J/mol×K	723.31	Joback Method
cpg	662.33	J/mol×K	756.19	Joback Method
cpg	677.46	J/mol×K	789.07	Joback Method
cpg	691.65	J/mol×K	821.95	Joback Method
cpg	704.91	J/mol×K	854.83	Joback Method
cpg	717.26	J/mol×K	887.72	Joback Method
dvisc	0.0015621	Pa×s	375.89	Joback Method
dvisc	0.0007200	Pa×s	428.31	Joback Method

dvisc	0.0003930	Pa×s	480.74	Joback Method
dvisc	0.0002416	Pa×s	533.16	Joback Method
dvisc	0.0001620	Pa×s	585.58	Joback Method
dvisc	0.0001161	Pa×s	638.01	Joback Method
dvisc	0.0000874	Pa×s	690.43	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U367909&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