Benzoic acid, 3-(3-methylbutyl)oxy-, 3-methylbutyl ester

Inchi: InChI=1S/C17H26O3/c1-13(2)8-10-19-16-7-5-6-15(12-16)17(18)20-11-9-14(3)4/h5-7,12-

InchiKey: HJSKFAIZIUUWEE-UHFFFAOYSA-N

Formula: C17H26O3

SMILES: CC(C)CCOC(=O)c1cccc(OCCC(C)C)c1

Mol. weight [g/mol]: 278.39

Physical Properties

Property code	Value	Unit	Source
gf	-148.76	kJ/mol	Joback Method
hf	-556.73	kJ/mol	Joback Method
hfus	30.37	kJ/mol	Joback Method
hvap	67.16	kJ/mol	Joback Method
log10ws	-4.70		Crippen Method
logp	4.314		Crippen Method
mcvol	239.940	ml/mol	McGowan Method
pc	1614.17	kPa	Joback Method
rinpol	2009.00		NIST Webbook
rinpol	2009.00		NIST Webbook
tb	717.85	K	Joback Method
tc	917.15	K	Joback Method
tf	384.68	K	Joback Method
vc	0.909	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	684.79	J/mol×K	717.85	Joback Method
cpg	702.32	J/mol×K	751.07	Joback Method
cpg	718.82	J/mol×K	784.28	Joback Method
cpg	734.30	J/mol×K	817.50	Joback Method
cpg	748.78	J/mol×K	850.72	Joback Method
cpg	762.28	J/mol×K	883.94	Joback Method
cpg	774.80	J/mol×K	917.15	Joback Method
dvisc	0.0013826	Pa×s	384.68	Joback Method

dvisc	0.0006173	Pa×s	440.21	Joback Method
dvisc	0.0003301	Pa×s	495.74	Joback Method
dvisc	0.0002003	Pa×s	551.26	Joback Method
dvisc	0.0001332	Pa×s	606.79	Joback Method
dvisc	0.0000948	Pa×s	662.32	Joback Method
dvisc	0.0000711	Pa×s	717.85	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375416&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
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