

Benzoic acid, 4-(3-methylbutyl)oxy-, 3-methylbutyl ester

Inchi:	InChI=1S/C17H26O3/c1-13(2)9-11-19-16-7-5-15(6-8-16)17(18)20-12-10-14(3)4/h5-8,13-
InchiKey:	QYQILGUQQBHAHE-UHFFFAOYSA-N
Formula:	C17H26O3
SMILES:	CC(C)CCOC(=O)c1ccc(OCCC(C)C)cc1
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
rinqol	2081.00		NIST Webbook
tb	717.85	K	Joback Method
tc	917.15	K	Joback Method
tf	384.68	K	Joback Method
vc	0.909	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	684.79	J/molxK	717.85	Joback Method
cpg	702.32	J/molxK	751.07	Joback Method
cpg	718.82	J/molxK	784.28	Joback Method
cpg	734.30	J/molxK	817.50	Joback Method
cpg	748.78	J/molxK	850.72	Joback Method
cpg	762.28	J/molxK	883.94	Joback Method
cpg	774.80	J/molxK	917.15	Joback Method
dvisc	0.0013826	Paxs	384.68	Joback Method
dvisc	0.0006173	Paxs	440.21	Joback Method

dvisc	0.0003301	Paxs	495.74	Joback Method
dvisc	0.0002003	Paxs	551.26	Joback Method
dvisc	0.0001332	Paxs	606.79	Joback Method
dvisc	0.0000948	Paxs	662.32	Joback Method
dvisc	0.0000711	Paxs	717.85	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375437&Units=SI
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

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

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