Benzoic acid, 3-methoxy-, 3-methylbutyl ester

Inchi: InChI=1S/C13H18O3/c1-10(2)7-8-16-13(14)11-5-4-6-12(9-11)15-3/h4-6,9-10H,7-8H2,1-3
InchiKey: UGYINAIOZICKRA-UHFFFAOYSA-N
Formula: C13H18O3
SMILES: COc1cccc(C(=O)OCCC(C)C)c1
Mol. weight [g/mol]: 222.28
CAS: 959013-88-8

Physical Properties

Property code	Value	Unit	Source
gf	-180.00	kJ/mol	Joback Method
hf	-468.89	kJ/mol	Joback Method
hfus	23.53	kJ/mol	Joback Method
hvap	58.65	kJ/mol	Joback Method
log10ws	-3.27		Crippen Method
logp	2.898		Crippen Method
mcvol	183.580	ml/mol	McGowan Method
pc	2239.76	kPa	Joback Method
rinpol	1694.00		NIST Webbook
rinpol	1694.00		NIST Webbook
tb	626.77	K	Joback Method
tc	832.59	K	Joback Method
tf	354.60	K	Joback Method
vc	0.692	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	469.86	J/mol×K	626.77	Joback Method
cpg	485.46	J/mol×K	661.07	Joback Method
cpg	500.22	J/mol×K	695.38	Joback Method
cpg	514.14	J/mol×K	729.68	Joback Method
cpg	527.21	J/mol×K	763.98	Joback Method
cpg	539.46	J/mol×K	798.29	Joback Method
cpg	550.88	J/mol×K	832.59	Joback Method

dvisc	0.0014954	Pa×s	354.60	Joback Method
dvisc	0.0007775	Pa×s	399.96	Joback Method
dvisc	0.0004619	Pa×s	445.32	Joback Method
dvisc	0.0003021	Pa×s	490.69	Joback Method
dvisc	0.0002123	Pa×s	536.05	Joback Method
dvisc	0.0001577	Pa×s	581.41	Joback Method
dvisc	0.0001222	Pa×s	626.77	Joback Method

Sources

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=C959013888&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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