

Benzoic acid,3-methyl, (2-methylpropyl)ester

Other names:	m-Toluic acid, 2-methylpropyl ester
Inchi:	InChI=1S/C12H16O2/c1-9(2)8-14-12(13)11-6-4-5-10(3)7-11/h4-7,9H,8H2,1-3H3
InchiKey:	DVLDXZFSLYUGHD-UHFFFAOYSA-N
Formula:	C12H16O2
SMILES:	<chem>Cc1cccc(C(=O)OCC(C)C)c1</chem>
Mol. weight [g/mol]:	192.25
CAS:	6640-78-4

Physical Properties

Property code	Value	Unit	Source
gf	-83.42	kJ/mol	Joback Method
hf	-316.03	kJ/mol	Joback Method
hfus	19.75	kJ/mol	Joback Method
hvap	54.01	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	2.808		Crippen Method
mcvol	163.620	ml/mol	McGowan Method
pc	2500.00	kPa	Joback Method
tb	581.47	K	Joback Method
tc	792.78	K	Joback Method
tf	321.10	K	Joback Method
vc	0.618	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.16	J/molxK	581.47	Joback Method
cpg	462.32	J/molxK	757.56	Joback Method
cpg	450.30	J/molxK	722.34	Joback Method
cpg	437.50	J/molxK	687.12	Joback Method
cpg	423.89	J/molxK	651.91	Joback Method
cpg	409.45	J/molxK	616.69	Joback Method
cpg	473.55	J/molxK	792.78	Joback Method
dvisc	0.0001687	Paxs	581.47	Joback Method

dvisc	0.0002174	Paxs	538.08	Joback Method
dvisc	0.0002929	Paxs	494.68	Joback Method
dvisc	0.0004180	Paxs	451.29	Joback Method
dvisc	0.0006432	Paxs	407.89	Joback Method
dvisc	0.0010969	Paxs	364.50	Joback Method
dvisc	0.0021607	Paxs	321.10	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6640784&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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