

Benzoic acid, 3-chloro, 3-methylbutyl ester

Inchi: InChI=1S/C12H15ClO2/c1-9(2)6-7-15-12(14)10-4-3-5-11(13)8-10/h3-5,8-9H,6-7H2,1-2H3
InchiKey: OAGLWNCLEPDCLB-UHFFFAOYSA-N
Formula: C12H15ClO2
SMILES: CC(C)CCOC(=O)c1cccc(Cl)c1
Mol. weight [g/mol]: 226.70

Physical Properties

Property code	Value	Unit	Source
gf	-95.35	kJ/mol	Joback Method
hf	-331.77	kJ/mol	Joback Method
hfus	23.95	kJ/mol	Joback Method
hvap	58.40	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	3.543		Crippen Method
mcvol	175.860	ml/mol	McGowan Method
pc	2410.00	kPa	Joback Method
ripol	1589.00		NIST Webbook
ripol	1586.00		NIST Webbook
ripol	1579.00		NIST Webbook
ripol	1586.00		NIST Webbook
ripol	1579.00		NIST Webbook
ripol	1570.00		NIST Webbook
ripol	1569.00		NIST Webbook
ripol	2102.00		NIST Webbook
ripol	2084.00		NIST Webbook
ripol	2123.00		NIST Webbook
ripol	2125.00		NIST Webbook
ripol	2092.00		NIST Webbook
ripol	2117.00		NIST Webbook
ripol	2084.00		NIST Webbook
ripol	2125.00		NIST Webbook
tb	618.90	K	Joback Method
tc	834.03	K	Joback Method
tf	351.02	K	Joback Method
vc	0.666	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	421.78	J/molxK	618.90	Joback Method
cpg	436.13	J/molxK	654.76	Joback Method
cpg	449.61	J/molxK	690.61	Joback Method
cpg	462.25	J/molxK	726.47	Joback Method
cpg	474.07	J/molxK	762.32	Joback Method
cpg	485.09	J/molxK	798.18	Joback Method
cpg	495.33	J/molxK	834.03	Joback Method
dvisc	0.0019039	Paxs	351.02	Joback Method
dvisc	0.0010010	Paxs	395.67	Joback Method
dvisc	0.0005996	Paxs	440.31	Joback Method
dvisc	0.0003947	Paxs	484.96	Joback Method
dvisc	0.0002788	Paxs	529.61	Joback Method
dvisc	0.0002079	Paxs	574.25	Joback Method
dvisc	0.0001617	Paxs	618.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R116993&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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