

Benzoic acid, 3,3-dimethylbut-2-yl ester

Inchi:	InChI=1S/C13H18O2/c1-10(13(2,3)4)15-12(14)11-8-6-5-7-9-11/h5-10H,1-4H3
InchiKey:	FDEANYZLSJVGGW-UHFFFAOYSA-N
Formula:	C13H18O2
SMILES:	CC(OC(=O)c1ccccc1)C(C)(C)C
Mol. weight [g/mol]:	206.28

Physical Properties

Property code	Value	Unit	Source
gf	-62.53	kJ/mol	Joback Method
hf	-333.95	kJ/mol	Joback Method
hfus	15.32	kJ/mol	Joback Method
hvap	54.28	kJ/mol	Joback Method
log10ws	-3.68		Crippen Method
logp	3.278		Crippen Method
mcvol	177.710	ml/mol	McGowan Method
pc	2351.92	kPa	Joback Method
rinqol	1446.00		NIST Webbook
tb	596.14	K	Joback Method
tc	815.50	K	Joback Method
tf	322.27	K	Joback Method
vc	0.662	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	446.87	J/molxK	596.14	Joback Method
cpg	463.94	J/molxK	632.70	Joback Method
cpg	479.86	J/molxK	669.26	Joback Method
cpg	494.71	J/molxK	705.82	Joback Method
cpg	508.52	J/molxK	742.38	Joback Method
cpg	521.35	J/molxK	778.94	Joback Method
cpg	533.25	J/molxK	815.50	Joback Method
dvisc	0.0032898	Paxs	322.27	Joback Method
dvisc	0.0014025	Paxs	367.91	Joback Method

dvisc	0.0007218	Paxs	413.56	Joback Method
dvisc	0.0004239	Paxs	459.20	Joback Method
dvisc	0.0002741	Paxs	504.85	Joback Method
dvisc	0.0001905	Paxs	550.50	Joback Method
dvisc	0.0001400	Paxs	596.14	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=U368207&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

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