

4-Butylbenzoic acid, oct-3-en-2-yl ester

Inchi:	InChI=1S/C19H28O2/c1-4-6-8-9-10-16(3)21-19(20)18-14-12-17(13-15-18)11-7-5-2/h9-10
InchiKey:	MBAMGAVULWQNEI-MDZDMXLPSA-N
Formula:	C19H28O2
SMILES:	CCCCC=CC(C)OC(=O)c1ccc(CCCC)cc1
Mol. weight [g/mol]:	288.42

Physical Properties

Property code	Value	Unit	Source
gf	55.74	kJ/mol	Joback Method
hf	-343.29	kJ/mol	Joback Method
hfus	38.08	kJ/mol	Joback Method
hvap	69.55	kJ/mol	Joback Method
log10ws	-6.25		Crippen Method
logp	5.321		Crippen Method
mcvol	257.950	ml/mol	McGowan Method
pc	1456.79	kPa	Joback Method
rinpol	2112.10		NIST Webbook
tb	745.79	K	Joback Method
tc	945.90	K	Joback Method
tf	394.91	K	Joback Method
vc	0.990	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	744.51	J/molxK	745.79	Joback Method
cpg	762.24	J/molxK	779.14	Joback Method
cpg	778.92	J/molxK	812.49	Joback Method
cpg	794.61	J/molxK	845.84	Joback Method
cpg	809.35	J/molxK	879.19	Joback Method
cpg	823.18	J/molxK	912.55	Joback Method
cpg	836.15	J/molxK	945.90	Joback Method
dvisc	0.0012732	Paxs	394.91	Joback Method
dvisc	0.0005694	Paxs	453.39	Joback Method

dvisc	0.0003060	Paxs	511.87	Joback Method
dvisc	0.0001868	Paxs	570.35	Joback Method
dvisc	0.0001250	Paxs	628.83	Joback Method
dvisc	0.0000896	Paxs	687.31	Joback Method
dvisc	0.0000676	Paxs	745.79	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292523&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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