

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: CCCC/C=C/C(C)OC(=O)c1ccc(CCCC)cc1
Mol. weight [g/mol]: 288.43

Physical Properties

Property code	Value	Unit	Source
hfus	38.08	kJ/mol	Joback Method
logp	5.321		Crippen Method
mcvol	257.950	ml/mol	McGowan Method
rinpol	2112.10		NIST Webbook
tf	264.01	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	744.51	J/mol×K	745.79	Joback Method
cpg	836.15	J/mol×K	945.90	Joback Method
cpg	823.18	J/mol×K	912.55	Joback Method
cpg	809.35	J/mol×K	879.19	Joback Method
cpg	794.61	J/mol×K	845.84	Joback Method
cpg	778.92	J/mol×K	812.49	Joback Method
cpg	762.24	J/mol×K	779.14	Joback Method
dvisc	0.0001868	Pa×s	570.35	Joback Method
dvisc	0.0000676	Pa×s	745.79	Joback Method
dvisc	0.0000896	Pa×s	687.31	Joback Method
dvisc	0.0001250	Pa×s	628.83	Joback Method
dvisc	0.0012732	Pa×s	394.91	Joback Method
dvisc	0.0003060	Pa×s	511.87	Joback Method
dvisc	0.0005694	Pa×s	453.39	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292523&Units=SI
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
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpola:	Non-polar retention indices
tf:	Normal melting (fusion) point

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