

4-Butylbenzoic acid, hexyl ester

Inchi:	InChI=1S/C17H26O2/c1-3-5-7-8-14-19-17(18)16-12-10-15(11-13-16)9-6-4-2/h10-13H,3-5
InchiKey:	FSMGSEAKDZNSAS-UHFFFAOYSA-N
Formula:	C17H26O2
SMILES:	CCCCCOC(=O)c1ccc(CCCC)cc1
Mol. weight [g/mol]:	262.39

Physical Properties

Property code	Value	Unit	Source
gf	-38.88	kJ/mol	Joback Method
hf	-413.95	kJ/mol	Joback Method
hfus	36.23	kJ/mol	Joback Method
hvap	65.53	kJ/mol	Joback Method
log10ws	-5.45		Crippen Method
logp	4.766		Crippen Method
mcvol	234.070	ml/mol	McGowan Method
pc	1615.47	kPa	Joback Method
rinpol	2009.50		NIST Webbook
rinpol	2009.50		NIST Webbook
tb	696.31	K	Joback Method
tc	890.56	K	Joback Method
tf	392.45	K	Joback Method
vc	0.903	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	654.61	J/molxK	696.31	Joback Method
cpg	671.96	J/molxK	728.69	Joback Method
cpg	688.36	J/molxK	761.06	Joback Method
cpg	703.83	J/molxK	793.44	Joback Method
cpg	718.39	J/molxK	825.81	Joback Method
cpg	732.07	J/molxK	858.19	Joback Method
cpg	744.91	J/molxK	890.56	Joback Method
dvisc	0.0013343	Paxs	392.45	Joback Method

dvisc	0.0006905	Paxs	443.09	Joback Method
dvisc	0.0004091	Paxs	493.74	Joback Method
dvisc	0.0002671	Paxs	544.38	Joback Method
dvisc	0.0001876	Paxs	595.02	Joback Method
dvisc	0.0001392	Paxs	645.67	Joback Method
dvisc	0.0001079	Paxs	696.31	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292323&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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